This journal is © The Royal Society of Chemistry 2014

Electronic Supplemental Information (ESI)

Comparison of shaking versus baking: Further understanding the energetics of a mechanochemical reaction

Kelley S. McKissic[a], Jeffery T. Caruso[a], Richard G. Blair[b] and James Mack[a]*

[a] *301 Clifton Court, Cincinnati, OH, USA. Fax: 01 513 556 9239 Tel: 01 513 556 9249 E-mail: james.mack@uc.edu*
[b] *4000 Central Florida Blvd , Orlando, FL, USA Town, Country. Fax: 01 407 823 2252; Tel: 01 407 823 0639; E-mail: Richard.blair@ucf.edu*

Table of Contents

Experimental 1

Analytical data of Products 9

Computational output files 10

This journal is © The Royal Society of Chemistry 2014

(15S) 9-methyl-9,10,11,15-tetrahydro-9,10-[3,4]furanoanthracene-12,14-dione-

One Stainless steel ball

9-methylanthracene (0.0971g, 0.5mmol), and maleic anhydride (0.0507g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch screw capped stainless steel vial inserted with a perfluoroelastomer O- ring, along with a 0.125 inch stainless steel ball bearing. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a white solid (0.0901g, 61.5%).

Two Stainless steel balls

9-methylanthracene (0.0973g, 0.5mmol), and maleic anhydride (0.0503g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch screw capped stainless steel vial inserted with a perfluoroelastomer O- ring, along with two 0.125 inch stainless steel ball bearings. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a white solid (0.1088g, 74.0%).

Three Stainless steel balls

9-methylanthracene (0.0954g, 0.5mmol), and maleic anhydride

This journal is © The Royal Society of Chemistry 2014

(0.0511g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch screw capped stainless steel vial inserted with a perfluoroelastomer O- ring, along with three 0.125 inch stainless steel ball bearings. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a white solid (0.0947g, 65.7%).

Four stainless steel balls

9-methylanthracene (0.0962g, 0.5mmol), and maleic anhydride (0.0491g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch screw capped stainless steel vial inserted with a perfluoroelastomer O- ring, along with four 0.125 inch stainless steel ball bearings. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a white solid (0.1241g, 85.4%)

One Teflon Ball

9-methylanthracene (0.1213g, 0.6mmol), and maleic anhydride (0.0624g, 0.6mmol), was added to a custom-made 2.0 x 0.5 inch Teflon vial, along with a 0.125 inch Teflon ball bearing. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a white solid (0.1023g, 55.8%).

Two Teflon Balls

This journal is © The Royal Society of Chemistry 2014

9-methylanthracene (0.0961g, 0.5mmol), and maleic anhydride (0.0490g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch Teflon vial, along with two 0.125 inch Teflon ball bearing. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a white solid (0.0980g, 67.6%).

Three Teflon Balls

9-methylanthracene (0.0954g, 0.5mmol), and maleic anhydride (0.0493g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch Teflon vial, along with three 0.125 inch Teflon ball bearings. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a white solid (0.0909g, 63.1%).

Four Teflon Balls

9-methylanthracene (0.0961g, 0.5mmol), and maleic anhydride (0.0491g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch Teflon vial, along with four 0.125 inch Teflon ball bearings. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a white solid (0.0837g, 57.2%).

This journal is © The Royal Society of Chemistry 2014

(15S)-12,14-dioxo-9,10,11,12,14,15-hexahydro-9,10-[3,4]furanoanthracene-9-carbaldehyde

One Stainless Steel ball

9-formylanthracene (0.1031g, 0.5mmol), and maleic anhydride (0.04905g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch screw capped stainless steel vial inserted with a perfluoroelastomer O- ring, along with a 0.125 inch stainless steel ball bearing. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a yellowish solid (0.0188g, 12.4%).

Two Stainless steel balls

9-formylanthracene (0.1040g, 0.5mmol), and maleic anhydride (0.0499g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch screw capped stainless steel vial inserted with a perfluoroelastomer O- ring, along with two 0.125 inch stainless steel ball bearings. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a yellowish solid (0.0125g, 8.1%).

Three Stainless steel balls

9-formylanthracene (0.1145g, 0.5mmol), and maleic anhydride (0.0540g,

This journal is © The Royal Society of Chemistry 2014

0.5mmol), was added to a custom-made 2.0 x 0.5 inch screw capped stainless steel vial inserted with a perfluoroelastomer O- ring, along with three 0.125 inch stainless steel ball bearings. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a yellowish solid (0.0174g, 10.3%).

Four stainless steel balls

9-formylanthracene (0.1040g, 0.5mmol), and maleic anhydride (0.0499g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch screw capped stainless steel vial inserted with a perfluoroelastomer O- ring, along with four 0.125 inch stainless steel ball bearings. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a yellowish solid (0.0125g, 8.1%).

One Teflon ball

9-formylanthracene (0.1314g, 0.6mmol), and maleic anhydride (0.0627g, 0.6mmol), was added to a custom-made 2.0 x 0.5 inch Teflon vial, along with a 0.125 inch Teflon ball bearing. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a yellowish solid (0.013g, 6.7%).

Two Teflon balls

9-formylanthracene (0.1018g, 0.5mmol), and maleic anhydride

This journal is © The Royal Society of Chemistry 2014

(0.0485g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch Teflon vial, along with two 0.125 inch Teflon ball bearing. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a yellowish solid (0.0119g, 7.9%).

Three Teflon Balls

9-formylanthracene (0.1109g, 0.5mmol), and maleic anhydride (0.0530g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch Teflon vial, along with three 0.125 inch Teflon ball bearing. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a yellowsih solid (0.0063g, 3.9%).

Four Teflon Balls

9-formylanthracene (0.1016g, 0.5mmol), and maleic anhydride (0.0480g, 0.5mmol), was added to a custom-made 2.0 x 0.5 inch Teflon vial, along with four 0.125 inch Teflon ball bearing. After placement of the vial in a Spex Certiprep 8000M mixer/mill, the reagents were ball milled for 16 hours. The resulting mixture was removed from the vial with ethyl acetate. The crude mixture was evaporated under reduced pressure and purified by column chromatography using a gradient cyclohexane-CH_2Cl_2 eluent to provide a yellowish solid (0.0092g, 6.5%).

This journal is © The Royal Society of Chemistry 2014

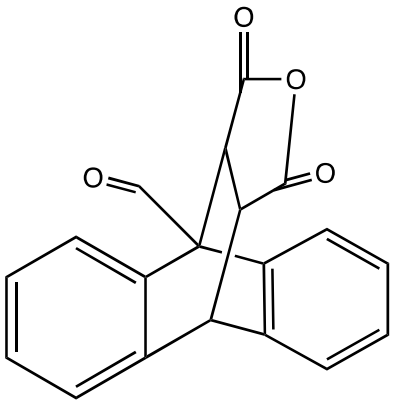
Solution experiment.

(15S) 9-methyl-9,10,11,15-tetrahydro-9,10-[3,4]furanoanthracene-12,14-dione-

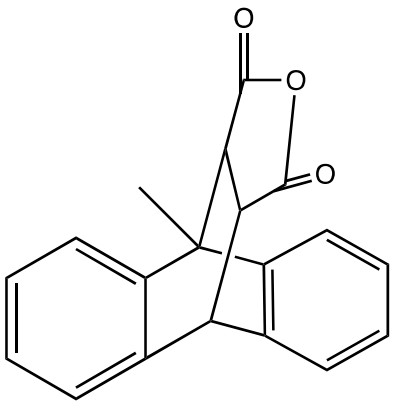
To a solution of 9-formylanthracene (0.1052g, 0.5mmol) in xylene, (10 mL) in a pressure vessel was added maleic anhydride (0.0500g, 0.5mmol). The mixture was stirred at 90 °C for 16.67 hrs. The crude mixture was evaporated under reduce pressure and purified by column chromatography using a gradient of cyclohexane-CH2Cl2 eluent to produce a yellowish solid (0.0259g, 16.7%)

This journal is © The Royal Society of Chemistry 2014

Using our methodology we synthesized the following compounds which have been synthesized previously; these molecules are consistent with literature reports



Yellowish solid, mp: (lit. 238-239 °C) ^{1}H NMR: δ 10.91 (s, 1H), 7.68 (d, 1H, 8 Hz), 7.48 (d, 1H, J = 8 Hz), 7.45 (m, 1H), 7.33-7.22 (m, 5H), 4.87 (d, J = 4 Hz), 4.09 (d, J = 12 Hz, 1H), 3.64 (d,d J = 12 Hz, J = 4 Hz, 1H)



White solid, mp: (lit.265.5-268 °C) ^{1}H NMR: δ 7.45 – 7.40 (m, 2H),

This journal is © The Royal Society of Chemistry 2014

7.38 – 7.34 (m, 2H), 7.29 – 7.23 (m, 4H), 4.82 (d, J = 4 Hz, 1H), 3.60 (d,d, J = 4 Hz, 8 Hz, 1H), 3.18 (d, J = 8 Hz, 1H), 2.31 (s, 3H)

Maleic Anhydride

```
Entering Gaussian System, Link 0=g03
 Initial command:
 /usr/local/g03d01/g03/l1.exe /tmp/pbstmp.6522862/Gau-6943.inp -
scrdir=/tmp/pbstmp.6522862/
 Entering Link 1 = /usr/local/g03d01/g03/l1.exe PID=      6944.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2004, Gaussian, Inc.
                   All Rights Reserved.

 This is the Gaussian(R) 03 program.  It is based on the
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,
 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be
 used, copied, transmitted, or stored only in accord with that
 written license.

 The following legend is applicable only to US Government
 contracts under FAR:

                       RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is
 subject to restrictions as set forth in subparagraphs (a)
 and (c) of the Commercial Computer Software - Restricted
 Rights clause in FAR 52.227-19.

 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ---------------------------------------------------------------
 Warning -- This program may not be used in any manner that
```

```
competes with the business of Gaussian, Inc. or will provide
assistance to any competitor of Gaussian, Inc.  The licensee
of this program is prohibited from giving any competitor of
Gaussian, Inc. access to this program.  By using this program,
the user acknowledges that Gaussian, Inc. is engaged in the
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.
-----------------------------------------------------------------


Cite this work as:
Gaussian 03, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

****************************************
Gaussian 03:  AM64L-G03RevD.01 13-Oct-2005
               18-Oct-2011
****************************************
%chk=maleic anhydride.chk
---------------------------------------
# opt b3lyp/6-31+g(d) geom=connectivity
---------------------------------------
1/14=-1,18=20,26=3,38=1,57=2/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20/3(3);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99//99;
```

```
 2/9=110/2;
 3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,74=-5/1,2,3;
 4/5=5,16=3/1;
 5/5=2,38=5/2;
 7//1,2,3,16;
 1/14=-1,18=20/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 ----------------
 maleic anhydride
 ----------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                     1.64225   1.60571   0.
 C                     0.56644   2.41127  -0.00029
 H                     2.69204   1.9022    0.00028
 H                     0.55508   3.50207  -0.00001
 C                    -0.71347   1.63139  -0.00113
 C                     1.25502   0.15789   0.
 O                    -1.87844   2.10722  -0.00248
 O                     2.04001  -0.82566  0.
 O                    -0.2807    0.15789   0.


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Initialization pass.
                           ----------------------------
                           !    Initial Parameters    !
                           ! (Angstroms and Degrees)  !
 --------------------------                            ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ------------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.344          estimate D2E/DX2
!
 ! R2    R(1,3)                  1.0909         estimate D2E/DX2
!
 ! R3    R(1,6)                  1.4987         estimate D2E/DX2
!
 ! R4    R(2,4)                  1.0909         estimate D2E/DX2
!
 ! R5    R(2,5)                  1.4988         estimate D2E/DX2
!
 ! R6    R(5,7)                  1.2584         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R7    R(5,9)                  1.5357         estimate D2E/DX2
!
 ! R8    R(6,8)                  1.2584         estimate D2E/DX2
!
 ! R9    R(6,9)                  1.5357         estimate D2E/DX2
!
 ! A1    A(2,1,3)              127.4035         estimate D2E/DX2
!
 ! A2    A(2,1,6)              111.8518         estimate D2E/DX2
!
 ! A3    A(3,1,6)              120.7447         estimate D2E/DX2
!
 ! A4    A(1,2,4)              127.4219         estimate D2E/DX2
!
 ! A5    A(1,2,5)              111.8196         estimate D2E/DX2
!
 ! A6    A(4,2,5)              120.7585         estimate D2E/DX2
!
 ! A7    A(2,5,7)              126.4274         estimate D2E/DX2
!
 ! A8    A(2,5,9)              104.9874         estimate D2E/DX2
!
 ! A9    A(7,5,9)              128.5853         estimate D2E/DX2
!
 ! A10   A(1,6,8)              126.4326         estimate D2E/DX2
!
 ! A11   A(1,6,9)              104.9736         estimate D2E/DX2
!
 ! A12   A(8,6,9)              128.5938         estimate D2E/DX2
!
 ! A13   A(5,9,6)              106.3677         estimate D2E/DX2
!
 ! D1    D(3,1,2,4)             -0.0188         estimate D2E/DX2
!
 ! D2    D(3,1,2,5)            179.9795         estimate D2E/DX2
!
 ! D3    D(6,1,2,4)            179.9769         estimate D2E/DX2
!
 ! D4    D(6,1,2,5)             -0.0248         estimate D2E/DX2
!
 ! D5    D(2,1,6,8)            179.9866         estimate D2E/DX2
!
 ! D6    D(2,1,6,9)             -0.0132         estimate D2E/DX2
!
 ! D7    D(3,1,6,8)             -0.0174         estimate D2E/DX2
!
 ! D8    D(3,1,6,9)            179.9828         estimate D2E/DX2
!
 ! D9    D(1,2,5,7)           -179.9478         estimate D2E/DX2
!
 ! D10   D(1,2,5,9)              0.0519         estimate D2E/DX2
!
```

```
 ! D11   D(4,2,5,7)              0.0506         estimate D2E/DX2
!
 ! D12   D(4,2,5,9)           -179.9497         estimate D2E/DX2
!
 ! D13   D(2,5,9,6)             -0.057          estimate D2E/DX2
!
 ! D14   D(7,5,9,6)            179.9427         estimate D2E/DX2
!
 ! D15   D(1,6,9,5)              0.0439         estimate D2E/DX2
!
 ! D16   D(8,6,9,5)           -179.9559         estimate D2E/DX2
!
 ---------------------------------------------------------------------
-----------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
 Number of steps in this run=  48 maximum allowed number of steps=
100.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.642251    1.605715    0.000000
    2          6             0        0.566435    2.411272   -0.000288
    3          1             0        2.692038    1.902203    0.000282
    4          1             0        0.555078    3.502068   -0.000006
    5          6             0       -0.713472    1.631391   -0.001130
    6          6             0        1.255023    0.157895    0.000000
    7          8             0       -1.878440    2.107223   -0.002478
    8          8             0        2.040006   -0.825656   -0.000003
    9          8             0       -0.280702    0.157895    0.000000
 ---------------------------------------------------------------------
                   Distance matrix (angstroms):
                    1          2          3          4          5
     1  C    0.000000
     2  C    1.343987   0.000000
     3  H    1.090852   2.185713   0.000000
     4  H    2.185887   1.090855   2.669488   0.000000
     5  C    2.355863   1.498792   3.416261   2.260233   0.000000
     6  C    1.498709   2.356239   2.260005   3.416638   2.458895
     7  O    3.556232   2.463710   4.575076   2.804926   1.258400
     8  O    2.463691   3.556559   2.804703   4.575391   3.690355
     9  O    2.407059   2.407353   3.446708   3.447031   1.535735
                    6          7          8          9
     6  C    0.000000
     7  O    3.690323   0.000000
     8  O    1.258400   4.894488   0.000000
     9  O    1.535725   2.520448   2.520527   0.000000
```

```
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.671864    1.215633    0.000562
    2          6             0       -0.672124    1.215835    0.000274
    3          1             0        1.334605    2.082081    0.000844
    4          1             0       -1.334883    2.082273    0.000556
    5          6             0       -1.229411   -0.175497   -0.000568
    6          6             0        1.229483   -0.175478    0.000562
    7          8             0       -2.447181   -0.492683   -0.001916
    8          8             0        2.447307   -0.492458    0.000559
    9          8             0        0.000049   -1.095773    0.000562
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      7.0442216      2.0858179
1.6092992
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       261.4497507290 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -379.269468240     A.U. after   12 cycles
             Convg  =    0.8626D-08             -V/T =  2.0115
             S**2   =   0.0000


*********************************************************************

            Population analysis using the SCF density.


*********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.24244 -19.21931 -19.21930 -10.38749 -
10.38748
 Alpha  occ. eigenvalues --  -10.27988 -10.27906  -1.10584  -1.08293
-1.03673
 Alpha  occ. eigenvalues --   -0.86570  -0.72350  -0.61843  -0.61413
-0.54180
 Alpha  occ. eigenvalues --   -0.49510  -0.48838  -0.48637  -0.46727
-0.43138
 Alpha  occ. eigenvalues --   -0.42473  -0.35367  -0.34521  -0.34026
-0.32588
 Alpha virt. eigenvalues --   -0.14902  -0.03087  -0.01993   0.00835
0.01135
 Alpha virt. eigenvalues --    0.01656   0.04135   0.05193   0.05318
0.06267
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.07474   0.07966   0.09294   0.09377
0.09768
 Alpha virt. eigenvalues --    0.11094   0.13249   0.13349   0.14804
0.16595
 Alpha virt. eigenvalues --    0.17047   0.19112   0.21136   0.22397
0.23074
 Alpha virt. eigenvalues --    0.25773   0.25930   0.26492   0.26853
0.28035
 Alpha virt. eigenvalues --    0.29530   0.30231   0.30537   0.33573
0.33945
 Alpha virt. eigenvalues --    0.34732   0.38104   0.39282   0.40499
0.51623
 Alpha virt. eigenvalues --    0.58753   0.60917   0.66210   0.66867
0.69863
 Alpha virt. eigenvalues --    0.70455   0.75215   0.77303   0.85164
0.85964
 Alpha virt. eigenvalues --    0.87727   0.96290   0.98557   1.02850
1.04774
 Alpha virt. eigenvalues --    1.08687   1.15560   1.18669   1.19515
1.20795
 Alpha virt. eigenvalues --    1.27045   1.29061   1.29514   1.29792
1.31040
 Alpha virt. eigenvalues --    1.32352   1.33803   1.35560   1.37945
1.39299
 Alpha virt. eigenvalues --    1.44877   1.48392   1.50413   1.59955
1.61781
 Alpha virt. eigenvalues --    1.66741   1.72625   1.73317   1.75692
1.77054
 Alpha virt. eigenvalues --    1.83529   1.86157   1.90634   1.91079
1.93027
 Alpha virt. eigenvalues --    1.99242   1.99461   2.07887   2.13076
2.13737
 Alpha virt. eigenvalues --    2.18004   2.28195   2.38638   2.38976
2.51291
 Alpha virt. eigenvalues --    2.55739   2.63336   2.67064   2.69686
2.69935
 Alpha virt. eigenvalues --    2.88023   2.89789   3.07947   3.09845
3.15442
 Alpha virt. eigenvalues --    4.06393   4.16417   4.17537   4.36888
4.37684
 Alpha virt. eigenvalues --    4.47581   4.72004
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C    6.143446  -0.359189   0.315486  -0.004296   0.180377  -
0.044206
     2  C   -0.359189   6.143622  -0.004320   0.315523  -0.044540
0.180298
     3  H    0.315486  -0.004320   0.455512  -0.001044  -0.001465  -
0.004793
     4  H   -0.004296   0.315523  -0.001044   0.455440  -0.004793  -
0.001484
```

This journal is © The Royal Society of Chemistry 2014

```
     5  C    0.180377  -0.044540  -0.001465  -0.004793   5.043547  -
0.059287
     6  C   -0.044206   0.180298  -0.004793  -0.001484  -0.059287
5.043178
     7  O   -0.026509  -0.118886  -0.000401  -0.001776   0.418614
0.023725
     8  O   -0.118892  -0.026535  -0.001773  -0.000401   0.023748
0.418587
     9  O   -0.107942  -0.107878   0.004671   0.004665   0.110989
0.111047
               7          8          9
     1  C   -0.026509  -0.118892  -0.107942
     2  C   -0.118886  -0.026535  -0.107878
     3  H   -0.000401  -0.001773   0.004671
     4  H   -0.001776  -0.000401   0.004665
     5  C    0.418614   0.023748   0.110989
     6  C    0.023725   0.418587   0.111047
     7  O    8.157599  -0.000039  -0.042545
     8  O   -0.000039   8.157665  -0.042550
     9  O   -0.042545  -0.042550   8.435617
 Mulliken atomic charges:
               1
     1  C    0.021726
     2  C    0.021904
     3  H    0.238127
     4  H    0.238166
     5  C    0.332809
     6  C    0.332935
     7  O   -0.409782
     8  O   -0.409810
     9  O   -0.366075
 Sum of Mulliken charges=   0.00000
 Atomic charges with hydrogens summed into heavy atoms:
               1
     1  C    0.259853
     2  C    0.260070
     3  H    0.000000
     4  H    0.000000
     5  C    0.332809
     6  C    0.332935
     7  O   -0.409782
     8  O   -0.409810
     9  O   -0.366075
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=   676.2202
 Charge=     0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=    -0.0003    Y=     4.4614    Z=     0.0021  Tot=     4.4614
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=   -50.0934   YY=   -37.0353   ZZ=   -38.4850
   XY=    -0.0026   XZ=    -0.0075   YZ=     0.0016
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
```

```
   XX=    -8.2222   YY=     4.8359   ZZ=     3.3863
   XY=    -0.0026   XZ=    -0.0075   YZ=     0.0016
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=    -0.0022  YYY=     8.9251  ZZZ=    -0.0043  XYY=    -0.0030
  XXY=    11.2713  XXZ=     0.0166  XZZ=     0.0005  YZZ=    -3.4004
  YYZ=     0.0041  XYZ=     0.0050
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=  -679.3568 YYYY=  -204.2585 ZZZZ=   -37.7701 XXXY=    -0.0092
 XXXZ=    -0.1868 YYYX=    -0.0107 YYYZ=    -0.0115 ZZZX=    -0.1235
 ZZZY=    -0.0237 XXYY=  -126.8318 XXZZ=   -99.6316 YYZZ=   -46.3561
 XXYZ=    -0.0104 YYXZ=    -0.0448 ZZXY=     0.0003
 N-N= 2.614497507290D+02 E-N=-1.409038004677D+03  KE=
3.749396214534D+02
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.002990451   -0.004912093    0.000007878
    2          6          -0.003927531   -0.004444408   -0.000004922
    3          1          -0.004761682   -0.002219091    0.000002904
    4          1          -0.000782745   -0.005207908   -0.000020203
    5          6          -0.036302278    0.002844104   -0.000014832
    6          6           0.012891936   -0.033993796   -0.000012148
    7          8           0.085473378   -0.053111850    0.000113641
    8          8          -0.075058205    0.067040713    0.000008669
    9          8           0.025457579    0.034004329   -0.000080987
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.085473378 RMS     0.030325682


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.099219136 RMS     0.028119600
 Search for a local minimum.
 Step number   1 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Second derivative matrix not updated -- first step.
     Eigenvalues ---    0.00448   0.00588   0.00610   0.01610
0.01636
     Eigenvalues ---    0.02160   0.16000   0.16000   0.22643
0.24694
     Eigenvalues ---    0.25000   0.25000   0.28333   0.28529
0.31449
     Eigenvalues ---    0.32337   0.34714   0.34714   0.54026
0.80209
     Eigenvalues ---
0.802091000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.00000
 RFO step:  Lambda=-5.40576919D-02.
 Linear search not attempted -- first point.
 Maximum step size (   0.300) exceeded in Quadratic search.
    -- Step size scaled by   0.863
 Iteration  1 RMS(Cart)=  0.07620364 RMS(Int)=  0.00193004
 Iteration  2 RMS(Cart)=  0.00234659 RMS(Int)=  0.00000986
 Iteration  3 RMS(Cart)=  0.00000513 RMS(Int)=  0.00000907
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000907
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.53977  -0.01534   0.00000  -0.02075  -0.02074
2.51903
    R2        2.06141  -0.00519   0.00000  -0.01115  -0.01115
2.05026
    R3        2.83215  -0.01467   0.00000  -0.03295  -0.03295
2.79920
    R4        2.06142  -0.00520   0.00000  -0.01118  -0.01118
2.05024
    R5        2.83231  -0.01468   0.00000  -0.03300  -0.03299
2.79931
    R6        2.37803  -0.09921   0.00000  -0.09998  -0.09998
2.27805
    R7        2.90212  -0.05769   0.00000  -0.14610  -0.14611
2.75601
    R8        2.37803  -0.09922   0.00000  -0.09999  -0.09999
2.27804
    R9        2.90210  -0.05768   0.00000  -0.14606  -0.14607
2.75603
    A1        2.22361   0.00788   0.00000   0.02365   0.02364
2.24725
    A2        1.95218  -0.01402   0.00000  -0.04031  -0.04029
1.91190
    A3        2.10739   0.00614   0.00000   0.01666   0.01665
2.12404
    A4        2.22393   0.00781   0.00000   0.02345   0.02344
2.24737
    A5        1.95162  -0.01390   0.00000  -0.03995  -0.03993
1.91169
    A6        2.10763   0.00609   0.00000   0.01650   0.01649
2.12412
    A7        2.20657   0.01202   0.00000   0.03360   0.03361
2.24018
    A8        1.83238   0.01604   0.00000   0.04649   0.04648
1.87885
    A9        2.24424  -0.02805   0.00000  -0.08009  -0.08009
2.16415
   A10        2.20667   0.01199   0.00000   0.03351   0.03351
2.24018
```

```
   A11        1.83214   0.01609   0.00000   0.04664   0.04664
1.87878
   A12        2.24438  -0.02807   0.00000  -0.08016  -0.08015
2.16423
   A13        1.85647  -0.00420   0.00000  -0.01287  -0.01291
1.84356
    D1       -0.00033   0.00001   0.00000   0.00006   0.00006  -
0.00027
    D2        3.14123   0.00001   0.00000   0.00011   0.00010
3.14134
    D3        3.14119   0.00001   0.00000   0.00011   0.00011
3.14130
    D4       -0.00043   0.00002   0.00000   0.00016   0.00015  -
0.00028
    D5        3.14136   0.00000   0.00000   0.00002   0.00002
3.14138
    D6       -0.00023   0.00000   0.00000   0.00001   0.00001  -
0.00022
    D7       -0.00030   0.00001   0.00000   0.00007   0.00007  -
0.00024
    D8        3.14129   0.00001   0.00000   0.00006   0.00006
3.14135
    D9       -3.14068  -0.00001   0.00000  -0.00007  -0.00007  -
3.14075
   D10        0.00091  -0.00002   0.00000  -0.00023  -0.00023
0.00068
   D11        0.00088   0.00000   0.00000  -0.00003  -0.00003
0.00085
   D12       -3.14071  -0.00001   0.00000  -0.00018  -0.00019  -
3.14090
   D13       -0.00099   0.00001   0.00000   0.00021   0.00021  -
0.00078
   D14        3.14059   0.00000   0.00000   0.00006   0.00006
3.14066
   D15        0.00077  -0.00001   0.00000  -0.00015  -0.00014
0.00062
   D16       -3.14082  -0.00001   0.00000  -0.00015  -0.00015  -
3.14097
         Item               Value     Threshold  Converged?
 Maximum Force            0.099219     0.000450     NO
 RMS     Force            0.028120     0.000300     NO
 Maximum Displacement     0.283640     0.001800     NO
 RMS     Displacement     0.076093     0.001200     NO
 Predicted change in Energy=-2.895254D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
```

This journal is © The Royal Society of Chemistry 2014

```
---------------------------------------------------------------------
   1          6             0        1.649226    1.624106    0.000035
   2          6             0        0.582106    2.422965   -0.000305
   3          1             0        2.699982    1.894347    0.000361
   4          1             0        0.545264    3.507277   -0.000097
   5          6             0       -0.651023    1.602151   -0.001041
   6          6             0        1.209340    0.209655   -0.000059
   7          8             0       -1.797528    1.974626   -0.002298
   8          8             0        1.889910   -0.785345   -0.000033
   9          8             0       -0.249060    0.200223   -0.000185
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  C    1.333013   0.000000
    3  H    1.084951   2.182851   0.000000
    4  H    2.182904   1.084938   2.691534   0.000000
    5  C    2.300355   1.481332   3.363721   2.249580   0.000000
    6  C    1.481274   2.300471   2.249489   3.363824   2.323790
    7  O    3.464532   2.421501   4.498227   2.799589   1.205492
    8  O    2.421442   3.464622   2.799458   4.498298   3.486615
    9  O    2.372958   2.373061   3.401015   3.401111   1.458415
                  6          7          8          9
    6  C    0.000000
    7  O    3.486600   0.000000
    8  O    1.205488   4.605936   0.000000
    9  O    1.458430   2.355050   2.355109   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
   1          6             0        0.666482    1.236689   -0.000054
   2          6             0       -0.666531    1.236785    0.000219
   3          1             0        1.345755    2.082684   -0.000276
   4          1             0       -1.345780    2.082783    0.000503
   5          6             0       -1.161887   -0.159269    0.000099
   6          6             0        1.161902   -0.159280    0.000014
   7          8             0       -2.302950   -0.548095   -0.000525
   8          8             0        2.302985   -0.548034   -0.000377
   9          8             0       -0.000006   -1.040749    0.000666
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.9399854      2.3356597
1.7475276
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
```

```
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       270.5471159463 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -379.301343309     A.U. after   12 cycles
             Convg  =    0.2336D-08             -V/T =  2.0097
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.004007931    0.000553889    0.000005133
    2          6          -0.000633712    0.003919349    0.000008282
    3          1          -0.001085967   -0.001243980    0.000001842
    4          1          -0.000885513   -0.001387792   -0.000015615
    5          6          -0.006633419   -0.017993448    0.000008503
    6          6          -0.015423664   -0.011427190    0.000001213
    7          8           0.014563261   -0.011789173    0.000031108
```

```
    8          8          -0.015420119    0.010642059    0.000005142
    9          8           0.021511201    0.028726286   -0.000045608
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.028726286 RMS     0.010117546


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.029586049 RMS     0.008633801
 Search for a local minimum.
 Step number   2 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2
 Trust test= 1.10D+00 RLast= 3.00D-01 DXMaxT set to 4.24D-01
     Eigenvalues ---    0.00442   0.00609   0.00633   0.01565
0.01647
     Eigenvalues ---    0.02172   0.15981   0.16000   0.21212
0.22687
     Eigenvalues ---    0.25000   0.25344   0.26280   0.28479
0.31352
     Eigenvalues ---    0.33285   0.34714   0.34741   0.54385
0.80209
     Eigenvalues ---
0.867411000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.00000
 RFO step:  Lambda=-3.70549570D-03.
 Quartic linear search produced a step of  0.34403.
 Iteration  1 RMS(Cart)=  0.04227931 RMS(Int)=  0.00086583
 Iteration  2 RMS(Cart)=  0.00113729 RMS(Int)=  0.00016401
 Iteration  3 RMS(Cart)=  0.00000028 RMS(Int)=  0.00016401
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.51903   0.00206  -0.00713   0.01527   0.00785
2.52688
    R2        2.05026  -0.00136  -0.00384   0.00024  -0.00359
2.04667
    R3        2.79920   0.00087  -0.01133   0.02100   0.00958
2.80878
    R4        2.05024  -0.00136  -0.00385   0.00027  -0.00357
2.04666
    R5        2.79931   0.00085  -0.01135   0.02094   0.00950
2.80881
    R6        2.27805  -0.01749  -0.03440   0.00996  -0.02443
2.25362
    R7        2.75601  -0.02959  -0.05027  -0.06174  -0.11178
2.64423
```

```
    R8        2.27804  -0.01749  -0.03440   0.00997  -0.02443
2.25362
    R9        2.75603  -0.02959  -0.05025  -0.06176  -0.11178
2.64425
    A1        2.24725   0.00412   0.00813   0.00920   0.01753
2.26478
    A2        1.91190  -0.00633  -0.01386  -0.00750  -0.02175
1.89015
    A3        2.12404   0.00221   0.00573  -0.00170   0.00422
2.12826
    A4        2.24737   0.00410   0.00806   0.00918   0.01744
2.26481
    A5        1.91169  -0.00629  -0.01374  -0.00745  -0.02158
1.89011
    A6        2.12412   0.00219   0.00567  -0.00172   0.00415
2.12827
    A7        2.24018   0.00697   0.01156   0.01840   0.02991
2.27009
    A8        1.87885   0.00135   0.01599  -0.01901  -0.00292
1.87594
    A9        2.16415  -0.00832  -0.02755   0.00061  -0.02700
2.13715
   A10        2.24018   0.00697   0.01153   0.01845   0.02993
2.27011
   A11        1.87878   0.00137   0.01605  -0.01900  -0.00285
1.87592
   A12        2.16423  -0.00834  -0.02758   0.00055  -0.02707
2.13716
   A13        1.84356   0.00990  -0.00444   0.05296   0.04911
1.89267
    D1       -0.00027   0.00000   0.00002   0.00004   0.00006  -
0.00021
    D2        3.14134   0.00001   0.00004   0.00002   0.00005
3.14139
    D3        3.14130   0.00000   0.00004  -0.00007  -0.00003
3.14127
    D4       -0.00028   0.00001   0.00005  -0.00009  -0.00004  -
0.00032
    D5        3.14138   0.00000   0.00001   0.00004   0.00004
3.14142
    D6       -0.00022   0.00000   0.00000   0.00026   0.00026
0.00004
    D7       -0.00024   0.00000   0.00002  -0.00006  -0.00004  -
0.00028
    D8        3.14135   0.00000   0.00002   0.00016   0.00018
3.14153
    D9       -3.14075  -0.00001  -0.00002  -0.00065  -0.00067  -
3.14142
   D10        0.00068  -0.00001  -0.00008  -0.00011  -0.00019
0.00049
   D11        0.00085  -0.00001  -0.00001  -0.00066  -0.00068
0.00018
```

```
   D12       -3.14090  -0.00001  -0.00006  -0.00013  -0.00019  -
3.14109
   D13       -0.00078   0.00001   0.00007   0.00024   0.00032  -
0.00046
   D14        3.14066   0.00001   0.00002   0.00075   0.00077
3.14142
   D15        0.00062  -0.00001  -0.00005  -0.00029  -0.00035
0.00028
   D16       -3.14097  -0.00001  -0.00005  -0.00008  -0.00015  -
3.14112
         Item               Value     Threshold  Converged?
 Maximum Force            0.029586     0.000450     NO
 RMS     Force            0.008634     0.000300     NO
 Maximum Displacement     0.150610     0.001800     NO
 RMS     Displacement     0.042683     0.001200     NO
 Predicted change in Energy=-5.592166D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.660689    1.635922    0.000042
    2          6             0        0.590193    2.437207   -0.000371
    3          1             0        2.714155    1.887324    0.000477
    4          1             0        0.534484    3.518821   -0.000186
    5          6             0       -0.629006    1.587022   -0.001183
    6          6             0        1.188620    0.226536   -0.000032
    7          8             0       -1.780697    1.896562   -0.001891
    8          8             0        1.810211   -0.791221    0.000082
    9          8             0       -0.210430    0.251830   -0.000560
 ---------------------------------------------------------------------
                    Distance matrix (angstroms):
                    1          2          3          4          5
     1  C    0.000000
     2  C    1.337168   0.000000
     3  H    1.083049   2.193989   0.000000
     4  H    2.194002   1.083048   2.722637   0.000000
     5  C    2.290218   1.486360   3.356623   2.255119   0.000000
     6  C    1.486344   2.290236   2.255101   3.356641   2.270394
     7  O    3.451243   2.431753   4.494863   2.826976   1.192564
     8  O    2.431745   3.451260   2.826963   4.494880   3.406732
     9  O    2.327401   2.327417   3.350827   3.350840   1.399265
                    6          7          8          9
     6  C    0.000000
     7  O    3.406734   0.000000
     8  O    1.192562   4.485399   0.000000
     9  O    1.399278   2.273958   2.273971   0.000000
 Stoichiometry    C4H2O3
```

This journal is © The Royal Society of Chemistry 2014

```
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.668580    1.255200   -0.000065
    2          6             0       -0.668588    1.255215    0.000105
    3          1             0        1.361312    2.087736   -0.000180
    4          1             0       -1.361325    2.087747    0.000344
    5          6             0       -1.135194   -0.156006   -0.000083
    6          6             0        1.135200   -0.156000    0.000078
    7          8             0       -2.242696   -0.598323   -0.000176
    8          8             0        2.242703   -0.598315   -0.000159
    9          8             0       -0.000003   -0.974104    0.000289
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8630489      2.4498366
1.8053855
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       274.5632915503 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
```

```
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -379.306128055     A.U. after   11 cycles
             Convg  =    0.5863D-08             -V/T =  2.0089
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.001692460    0.002454710    0.000015606
    2          6           0.001869922    0.002300011   -0.000012705
    3          1          -0.000207421    0.000115534    0.000004783
    4          1           0.000170314   -0.000166515   -0.000013011
    5          6           0.008864542   -0.007220099    0.000067572
    6          6          -0.009435439    0.006468823   -0.000037135
    7          8          -0.010622910    0.003571655   -0.000020524
    8          8           0.006420022   -0.009185116    0.000016655
    9          8           0.001248509    0.001660998   -0.000021241
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.010622910 RMS     0.004450902


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.011185899 RMS     0.002685336
 Search for a local minimum.
 Step number   3 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3
 Trust test= 8.56D-01 RLast= 1.84D-01 DXMaxT set to 5.51D-01
     Eigenvalues ---    0.00428   0.00619   0.00645   0.01547
0.01658
     Eigenvalues ---    0.02185   0.16000   0.16012   0.22714
0.23614
     Eigenvalues ---    0.25000   0.25208   0.26486   0.28484
0.31298
     Eigenvalues ---    0.34059   0.34714   0.34774   0.54299
0.80209
     Eigenvalues ---
1.023691000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.00000
 RFO step:  Lambda=-3.20083935D-04.
 Quartic linear search produced a step of -0.02053.
 Iteration  1 RMS(Cart)=  0.00319577 RMS(Int)=  0.00000785
 Iteration  2 RMS(Cart)=  0.00000455 RMS(Int)=  0.00000568
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000568
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.52688  -0.00022  -0.00016  -0.00077  -0.00092
2.52596
    R2        2.04667  -0.00017   0.00007  -0.00085  -0.00078
2.04589
    R3        2.80878   0.00283  -0.00020   0.00743   0.00724
2.81602
    R4        2.04666  -0.00018   0.00007  -0.00085  -0.00078
2.04588
    R5        2.80881   0.00283  -0.00020   0.00741   0.00722
2.81603
    R6        2.25362   0.01119   0.00050   0.01054   0.01104
2.26466
    R7        2.64423  -0.00135   0.00229  -0.01030  -0.00801
2.63622
    R8        2.25362   0.01119   0.00050   0.01053   0.01104
2.26465
    R9        2.64425  -0.00135   0.00229  -0.01031  -0.00802
2.63623
    A1        2.26478   0.00012  -0.00036   0.00097   0.00060
2.26538
    A2        1.89015  -0.00056   0.00045  -0.00347  -0.00301
1.88714
    A3        2.12826   0.00044  -0.00009   0.00250   0.00241
2.13067
    A4        2.26481   0.00011  -0.00036   0.00094   0.00057
2.26538
    A5        1.89011  -0.00055   0.00044  -0.00342  -0.00296
1.88715
    A6        2.12827   0.00044  -0.00009   0.00248   0.00239
2.13066
    A7        2.27009  -0.00093  -0.00061  -0.00216  -0.00277
2.26733
    A8        1.87594   0.00031   0.00006   0.00270   0.00276
1.87870
    A9        2.13715   0.00063   0.00055  -0.00055   0.00001
2.13716
   A10        2.27011  -0.00093  -0.00061  -0.00216  -0.00278
2.26733
   A11        1.87592   0.00031   0.00006   0.00273   0.00278
1.87870
```

```
   A12        2.13716   0.00062   0.00056  -0.00056   0.00000
2.13715
   A13        1.89267   0.00050  -0.00101   0.00146   0.00043
1.89309
    D1       -0.00021   0.00001   0.00000   0.00016   0.00016  -
0.00005
    D2        3.14139   0.00001   0.00000   0.00064   0.00064  -
3.14116
    D3        3.14127   0.00001   0.00000   0.00054   0.00054  -
3.14138
    D4       -0.00032   0.00002   0.00000   0.00103   0.00102
0.00070
    D5        3.14142   0.00000   0.00000   0.00109   0.00109  -
3.14067
    D6        0.00004  -0.00001  -0.00001   0.00032   0.00031
0.00035
    D7       -0.00028   0.00001   0.00000   0.00144   0.00144
0.00116
    D8        3.14153   0.00000   0.00000   0.00066   0.00066  -
3.14100
    D9       -3.14142   0.00001   0.00001   0.00097   0.00098  -
3.14044
   D10        0.00049  -0.00002   0.00000  -0.00203  -0.00202  -
0.00153
   D11        0.00018   0.00001   0.00001   0.00140   0.00142
0.00159
   D12       -3.14109  -0.00001   0.00000  -0.00159  -0.00159
3.14051
   D13       -0.00046   0.00001  -0.00001   0.00220   0.00220
0.00173
   D14        3.14142  -0.00001  -0.00002  -0.00051  -0.00053
3.14089
   D15        0.00028   0.00000   0.00001  -0.00160  -0.00159  -
0.00132
   D16       -3.14112  -0.00001   0.00000  -0.00231  -0.00231
3.13976
         Item               Value     Threshold  Converged?
 Maximum Force            0.011186     0.000450     NO
 RMS     Force            0.002685     0.000300     NO
 Maximum Displacement     0.008747     0.001800     NO
 RMS     Displacement     0.003194     0.001200     NO
 Predicted change in Energy=-1.608463D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.662411    1.638620    0.000098
```

This journal is © The Royal Society of Chemistry 2014

```
   2          6             0        0.592293    2.439598   -0.000428
   3          1             0        2.715624    1.889309    0.000537
   4          1             0        0.535970    3.520768   -0.000489
   5          6             0       -0.627499    1.583591   -0.000281
   6          6             0        1.184900    0.227025   -0.000389
   7          8             0       -1.784894    1.894406   -0.001674
   8          8             0        1.809314   -0.795850    0.000683
   9          8             0       -0.209900    0.252537   -0.001679
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  C    1.336682   0.000000
    3  H    1.082637   2.193480   0.000000
    4  H    2.193479   1.082636   2.722600   0.000000
    5  C    2.290571   1.490181   3.357072   2.259715   0.000000
    6  C    1.490173   2.290559   2.259714   3.357060   2.263859
    7  O    3.456782   2.438904   4.500522   2.833984   1.198404
    8  O    2.438898   3.456771   2.833986   4.500511   3.405848
    9  O    2.329544   2.329539   3.352271   3.352261   1.395025
                  6          7          8          9
    6  C    0.000000
    7  O    3.405853   0.000000
    8  O    1.198402   4.489523   0.000000
    9  O    1.395034   2.275157   2.275159   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
   1          6             0       -0.668348    1.259184    0.000131
   2          6             0        0.668334    1.259186    0.000083
   3          1             0       -1.361309    2.090995    0.000312
   4          1             0        1.361291    2.090997    0.000169
   5          6             0        1.131930   -0.157047   -0.000812
   6          6             0       -1.131929   -0.157047    0.000267
   7          8             0        2.244765   -0.601760   -0.000070
   8          8             0       -2.244758   -0.601772   -0.000499
   9          8             0        0.000006   -0.972425    0.000756
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8301402      2.4485269
1.8023908
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
```

This journal is © The Royal Society of Chemistry 2014

```
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       274.2898418482 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -379.306304378     A.U. after   13 cycles
             Convg  =    0.2529D-08             -V/T =  2.0090
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.000676856   -0.000055901   -0.000038093
    2          6          -0.000247287    0.000633755    0.000131000
    3          1           0.000053567   -0.000074203   -0.000010420
    4          1          -0.000086052    0.000031883    0.000012026
    5          6           0.000159183   -0.001286079   -0.000376594
    6          6          -0.001281985   -0.000212708    0.000080130
    7          8          -0.001061193    0.000913700    0.000120539
    8          8           0.001176879   -0.000762435   -0.000044126
    9          8           0.000610031    0.000811988    0.000125538
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.001286079 RMS     0.000592142
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.001263923 RMS     0.000415962
 Search for a local minimum.
 Step number   4 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3  4
 Trust test= 1.10D+00 RLast= 2.38D-02 DXMaxT set to 5.51D-01
     Eigenvalues ---    0.00428   0.00621   0.00645   0.01544
0.01656
     Eigenvalues ---    0.02184   0.16000   0.16035   0.22079
0.22717
     Eigenvalues ---    0.24793   0.25000   0.28482   0.28618
0.31292
     Eigenvalues ---    0.33641   0.34714   0.34784   0.54983
0.80209
     Eigenvalues ---
0.920721000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.00000
 RFO step:  Lambda=-1.85926982D-05.
 Quartic linear search produced a step of  0.10874.
 Iteration  1 RMS(Cart)=  0.00309299 RMS(Int)=  0.00003432
 Iteration  2 RMS(Cart)=  0.00002173 RMS(Int)=  0.00002572
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00002572
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.52596   0.00073  -0.00010   0.00137   0.00127
2.52724
    R2        2.04589   0.00003  -0.00008   0.00009   0.00000
2.04589
    R3        2.81602   0.00034   0.00079   0.00042   0.00120
2.81722
    R4        2.04588   0.00004  -0.00008   0.00009   0.00001
2.04589
    R5        2.81603   0.00034   0.00079   0.00041   0.00120
2.81724
    R6        2.26466   0.00126   0.00120   0.00046   0.00166
2.26632
    R7        2.63622   0.00006  -0.00087  -0.00016  -0.00102
2.63519
    R8        2.26465   0.00126   0.00120   0.00047   0.00167
2.26632
    R9        2.63623   0.00005  -0.00087  -0.00017  -0.00105
2.63519
```

This journal is © The Royal Society of Chemistry 2014

A1	2.26538	0.00008	0.00007	0.00055	0.00062
2.26600					
A2	1.88714	0.00001	-0.00033	0.00022	-0.00012
1.88702					
A3	2.13067	-0.00009	0.00026	-0.00077	-0.00050
2.13017					
A4	2.26538	0.00008	0.00006	0.00056	0.00061
2.26599					
A5	1.88715	0.00001	-0.00032	0.00020	-0.00011
1.88703					
A6	2.13066	-0.00009	0.00026	-0.00076	-0.00050
2.13016					
A7	2.26733	-0.00053	-0.00030	-0.00193	-0.00232
2.26501					
A8	1.87870	-0.00031	0.00030	-0.00117	-0.00093
1.87776					
A9	2.13716	0.00084	0.00000	0.00315	0.00306
2.14022					
A10	2.26733	-0.00053	-0.00030	-0.00195	-0.00224
2.26509					
A11	1.87870	-0.00031	0.00030	-0.00118	-0.00090
1.87780					
A12	2.13715	0.00084	0.00000	0.00313	0.00314
2.14030					
A13	1.89309	0.00060	0.00005	0.00196	0.00200
1.89509					
D1	-0.00005	-0.00001	0.00002	-0.00028	-0.00026	-
0.00031					
D2	-3.14116	-0.00004	0.00007	-0.00294	-0.00287
3.13916					
D3	-3.14138	-0.00003	0.00006	-0.00189	-0.00183
3.13998					
D4	0.00070	-0.00006	0.00011	-0.00455	-0.00444	-
0.00374					
D5	-3.14067	0.00000	0.00012	-0.00323	-0.00311
3.13940					
D6	0.00035	0.00002	0.00003	-0.00393	-0.00390	-
0.00355					
D7	0.00116	-0.00003	0.00016	-0.00469	-0.00453	-
0.00337					
D8	-3.14100	-0.00001	0.00007	-0.00539	-0.00532
3.13687					
D9	-3.14044	-0.00007	0.00011	-0.01244	-0.01232
3.13043					
D10	-0.00153	0.00009	-0.00022	0.01158	0.01135
0.00982					
D11	0.00159	-0.00009	0.00015	-0.01486	-0.01468	-
0.01309					
D12	3.14051	0.00006	-0.00017	0.00916	0.00898	-
3.13370					
D13	0.00173	-0.00007	0.00024	-0.01394	-0.01372	-
0.01199					

```
   D14        3.14089   0.00006  -0.00006   0.00788   0.00787  -
3.13443
   D15       -0.00132   0.00004  -0.00017   0.01126   0.01110
0.00979
   D16        3.13976   0.00006  -0.00025   0.01062   0.01038  -
3.13305
         Item               Value     Threshold  Converged?
 Maximum Force            0.001264     0.000450     NO
 RMS     Force            0.000416     0.000300     NO
 Maximum Displacement     0.013026     0.001800     NO
 RMS     Displacement     0.003092     0.001200     NO
 Predicted change in Energy=-1.111467D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.662584    1.638292    0.000080
    2          6             0        0.591921    2.439667   -0.000952
    3          1             0        2.715951    1.888332    0.002030
    4          1             0        0.534925    3.520804    0.000185
    5          6             0       -0.628277    1.583153   -0.007174
    6          6             0        1.184704    0.226154   -0.000132
    7          8             0       -1.785832    1.896670    0.000425
    8          8             0        1.811753   -0.796143   -0.001469
    9          8             0       -0.209511    0.253075    0.003385
 ---------------------------------------------------------------------
                   Distance matrix (angstroms):
                    1          2          3          4          5
     1  C    0.000000
     2  C    1.337356   0.000000
     3  H    1.082638   2.194421   0.000000
     4  H    2.194417   1.082639   2.724305   0.000000
     5  C    2.291536   1.490818   3.358137   2.259996   0.000000
     6  C    1.490806   2.291513   2.259991   3.358114   2.264597
     7  O    3.458082   2.438966   4.501791   2.832618   1.199284
     8  O    2.439001   3.458100   2.832666   4.501813   3.408054
     9  O    2.328858   2.328840   3.351477   3.351454   1.394484
                    6          7          8          9
     6  C    0.000000
     7  O    3.408036   0.000000
     8  O    1.199284   4.493759   0.000000
     9  O    1.394480   2.277323   2.277365   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
```

This journal is © The Royal Society of Chemistry 2014

```
 Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.668673    1.258786   -0.001009
    2          6             0        0.668683    1.258770   -0.000237
    3          1             0       -1.362140    2.090173   -0.003152
    4          1             0        1.362165    2.090146   -0.001838
    5          6             0        1.132293   -0.158114    0.006454
    6          6             0       -1.132295   -0.158097   -0.000148
    7          8             0        2.246869   -0.600769   -0.001187
    8          8             0       -2.246888   -0.600773    0.001580
    9          8             0        0.000010   -0.972006   -0.003564
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8369818      2.4444967
1.8006909
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       274.1992809778 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
```

```
 SCF Done:  E(RB+HF-LYP) =  -379.306289918     A.U. after   10 cycles
             Convg  =    0.5399D-08             -V/T =  2.0090
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000034813    0.000121793    0.000013255
    2          6           0.000131068    0.000006436   -0.000924449
    3          1           0.000029589   -0.000027644    0.000084923
    4          1          -0.000035215    0.000020768   -0.000070040
    5          6          -0.000249987    0.000052786    0.002794599
    6          6           0.000119526   -0.000234217    0.000047685
    7          8           0.000338594   -0.000068532   -0.000947248
    8          8          -0.000168570    0.000317808    0.000065033
    9          8          -0.000130193   -0.000189197   -0.001063760
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.002794599 RMS     0.000643617


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000675274 RMS     0.000267890
 Search for a local minimum.
 Step number   5 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3  5  4

 Trust test=-1.30D+00 RLast= 3.48D-02 DXMaxT set to 2.75D-01
 Energy Rises -- skip Quadratic search.
 Quartic linear search produced a step of -0.69766.
 Iteration  1 RMS(Cart)=  0.00215529 RMS(Int)=  0.00001218
 Iteration  2 RMS(Cart)=  0.00001073 RMS(Int)=  0.00000543
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000543
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.52724  -0.00011  -0.00089   0.00000  -0.00089
2.52635
    R2        2.04589   0.00002   0.00000   0.00000   0.00000
2.04589
    R3        2.81722   0.00006  -0.00083   0.00000  -0.00083
2.81638
    R4        2.04589   0.00002   0.00000   0.00000   0.00000
2.04589
    R5        2.81724   0.00005  -0.00084   0.00000  -0.00084
2.81639
    R6        2.26632  -0.00035  -0.00116   0.00000  -0.00116
2.26516
```

This journal is © The Royal Society of Chemistry 2014

R7	2.63519	0.00003	0.00071	0.00000	0.00071
2.63590					
R8	2.26632	-0.00036	-0.00116	0.00000	-0.00116
2.26516					
R9	2.63519	0.00003	0.00073	0.00000	0.00073
2.63592					
A1	2.26600	0.00005	-0.00043	0.00000	-0.00044
2.26557					
A2	1.88702	-0.00002	0.00009	0.00000	0.00009
1.88711					
A3	2.13017	-0.00002	0.00035	0.00000	0.00035
2.13051					
A4	2.26599	0.00005	-0.00043	0.00000	-0.00043
2.26557					
A5	1.88703	-0.00003	0.00008	0.00000	0.00008
1.88711					
A6	2.13016	-0.00002	0.00035	0.00000	0.00035
2.13051					
A7	2.26501	-0.00007	0.00162	0.00000	0.00164
2.26664					
A8	1.87776	0.00011	0.00065	0.00000	0.00066
1.87843					
A9	2.14022	-0.00003	-0.00214	0.00000	-0.00212
2.13811					
A10	2.26509	-0.00008	0.00156	0.00000	0.00156
2.26665					
A11	1.87780	0.00011	0.00063	0.00000	0.00063
1.87843					
A12	2.14030	-0.00003	-0.00219	0.00000	-0.00220
2.13810					
A13	1.89509	-0.00017	-0.00139	0.00000	-0.00139
1.89370					
D1	-0.00031	0.00007	0.00018	0.00000	0.00018	-
0.00013					
D2	3.13916	0.00020	0.00200	0.00000	0.00200
3.14116					
D3	3.13998	0.00022	0.00127	0.00000	0.00127
3.14126					
D4	-0.00374	0.00035	0.00310	0.00000	0.00310	-
0.00064					
D5	3.13940	-0.00013	0.00217	0.00000	0.00217
3.14157					
D6	-0.00355	0.00000	0.00272	0.00000	0.00272	-
0.00083					
D7	-0.00337	0.00001	0.00316	0.00000	0.00316	-
0.00021					
D8	3.13687	0.00014	0.00371	0.00000	0.00371
3.14058					
D9	3.13043	0.00056	0.00859	0.00000	0.00859
3.13902					
D10	0.00982	-0.00060	-0.00792	0.00000	-0.00792
0.00190					

```
   D11       -0.01309   0.00068   0.01024   0.00000   0.01024  -
0.00285
   D12       -3.13370  -0.00048  -0.00627   0.00000  -0.00626  -
3.13996
   D13       -0.01199   0.00059   0.00957   0.00000   0.00957  -
0.00241
   D14       -3.13443  -0.00046  -0.00549   0.00000  -0.00550  -
3.13993
   D15        0.00979  -0.00039  -0.00775   0.00000  -0.00775
0.00204
   D16       -3.13305  -0.00026  -0.00724   0.00000  -0.00724  -
3.14029
         Item               Value     Threshold  Converged?
 Maximum Force            0.000675     0.000450     NO
 RMS     Force            0.000268     0.000300     YES
 Maximum Displacement     0.009089     0.001800     NO
 RMS     Displacement     0.002157     0.001200     NO
 Predicted change in Energy=-3.343879D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.662463    1.638521    0.000092
    2          6             0        0.592182    2.439622   -0.000586
    3          1             0        2.715723    1.889013    0.000987
    4          1             0        0.535658    3.520782   -0.000283
    5          6             0       -0.627734    1.583462   -0.002364
    6          6             0        1.184841    0.226760   -0.000311
    7          8             0       -1.785186    1.895092   -0.001041
    8          8             0        1.810056   -0.795939    0.000032
    9          8             0       -0.209785    0.252692   -0.000147
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1          2          3          4          5
     1  C    0.000000
     2  C    1.336886   0.000000
     3  H    1.082638   2.193764   0.000000
     4  H    2.193763   1.082637   2.723115   0.000000
     5  C    2.290861   1.490372   3.357392   2.259799   0.000000
     6  C    1.490366   2.290852   2.259798   3.357382   2.264084
     7  O    3.457184   2.438933   4.500914   2.833582   1.198670
     8  O    2.438930   3.457177   2.833585   4.500908   3.406520
     9  O    2.329342   2.329338   3.352036   3.352029   1.394861
                       6          7          8          9
     6  C    0.000000
     7  O    3.406523   0.000000
     8  O    1.198669   4.490815   0.000000
```

```
    9  O    1.394867   2.275823   2.275826   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.668448    1.259064   -0.000213
    2          6             0        0.668438    1.259065   -0.000014
    3          1             0       -1.361563    2.090746   -0.000734
    4          1             0        1.361552    2.090747   -0.000440
    5          6             0        1.132042   -0.157367    0.001383
    6          6             0       -1.132041   -0.157365    0.000142
    7          8             0        2.245410   -0.601460   -0.000406
    8          8             0       -2.245405   -0.601469    0.000130
    9          8             0        0.000004   -0.972305   -0.000551
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8321953      2.4472990
1.8018685
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       274.2621545859 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -379.306307722     A.U. after   10 cycles
            Convg  =    0.4574D-08             -V/T =  2.0090
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.000460900   -0.000002355   -0.000022444
    2          6          -0.000134058    0.000441819   -0.000187599
    3          1           0.000046329   -0.000060273    0.000018421
    4          1          -0.000070710    0.000028403   -0.000012837
    5          6           0.000032333   -0.000882643    0.000580805
    6          6          -0.000858489   -0.000220080    0.000071689
    7          8          -0.000632229    0.000615475   -0.000200704
    8          8           0.000769291   -0.000433993   -0.000012085
    9          8           0.000386634    0.000513647   -0.000235246
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000882643 RMS     0.000405937


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000771533 RMS     0.000274333
 Search for a local minimum.
 Step number   6 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3  5  4
                                                             6
     Eigenvalues ---    0.00469   0.00613   0.01309   0.01656
0.02135
     Eigenvalues ---    0.04722   0.14671   0.16000   0.17538
0.22717
     Eigenvalues ---    0.24022   0.25000   0.26945   0.28482
0.31292
     Eigenvalues ---    0.33423   0.34714   0.34751   0.53457
0.80209
     Eigenvalues ---
0.928241000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.00000
 RFO step:  Lambda=-1.58697684D-05.
```

This journal is © The Royal Society of Chemistry 2014

```
 Quartic linear search produced a step of  0.00004.
 Iteration  1 RMS(Cart)=  0.00225882 RMS(Int)=  0.00001225
 Iteration  2 RMS(Cart)=  0.00000743 RMS(Int)=  0.00000874
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000874
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.52635   0.00048   0.00000   0.00178   0.00178
2.52813
    R2        2.04589   0.00003   0.00000   0.00004   0.00004
2.04593
    R3        2.81638   0.00025   0.00000   0.00101   0.00101
2.81739
    R4        2.04589   0.00003   0.00000   0.00005   0.00005
2.04593
    R5        2.81639   0.00025   0.00000   0.00099   0.00099
2.81739
    R6        2.26516   0.00077   0.00000   0.00097   0.00097
2.26613
    R7        2.63590   0.00005   0.00000  -0.00116  -0.00116
2.63475
    R8        2.26516   0.00077   0.00000   0.00098   0.00098
2.26613
    R9        2.63592   0.00004   0.00000  -0.00117  -0.00117
2.63475
    A1        2.26557   0.00007   0.00000   0.00099   0.00099
2.26656
    A2        1.88711   0.00000   0.00000  -0.00006  -0.00006
1.88704
    A3        2.13051  -0.00007   0.00000  -0.00093  -0.00093
2.12959
    A4        2.26557   0.00007   0.00000   0.00099   0.00100
2.26656
    A5        1.88711   0.00000   0.00000  -0.00008  -0.00008
1.88703
    A6        2.13051  -0.00007   0.00000  -0.00092  -0.00091
2.12959
    A7        2.26664  -0.00039   0.00000  -0.00311  -0.00312
2.26352
    A8        1.87843  -0.00018   0.00000  -0.00118  -0.00119
1.87724
    A9        2.13811   0.00058   0.00000   0.00433   0.00432
2.14242
   A10        2.26665  -0.00039   0.00000  -0.00312  -0.00314
2.26351
   A11        1.87843  -0.00019   0.00000  -0.00119  -0.00121
1.87722
   A12        2.13810   0.00058   0.00000   0.00432   0.00431
2.14241
   A13        1.89370   0.00037   0.00000   0.00254   0.00254
1.89624
```

```
    D1       -0.00013   0.00001   0.00000   0.00013   0.00013
0.00000
    D2        3.14116   0.00004   0.00000  -0.00032  -0.00032
3.14084
    D3        3.14126   0.00004   0.00000  -0.00013  -0.00013
3.14112
    D4       -0.00064   0.00006   0.00000  -0.00058  -0.00058  -
0.00122
    D5        3.14157  -0.00004   0.00000  -0.00578  -0.00576
3.13581
    D6       -0.00083   0.00001   0.00000   0.00460   0.00460
0.00376
    D7       -0.00021  -0.00002   0.00000  -0.00601  -0.00600  -
0.00621
    D8        3.14058   0.00004   0.00000   0.00436   0.00436  -
3.13825
    D9        3.13902   0.00012   0.00000   0.00476   0.00475  -
3.13942
   D10        0.00190  -0.00012   0.00000  -0.00362  -0.00362  -
0.00171
   D11       -0.00285   0.00014   0.00000   0.00434   0.00434
0.00149
   D12       -3.13996  -0.00010   0.00000  -0.00403  -0.00402
3.13920
   D13       -0.00241   0.00013   0.00000   0.00650   0.00651
0.00410
   D14       -3.13993  -0.00009   0.00000  -0.00109  -0.00111  -
3.14104
   D15        0.00204  -0.00009   0.00000  -0.00685  -0.00686  -
0.00482
   D16       -3.14029  -0.00004   0.00000   0.00259   0.00261  -
3.13768
         Item               Value     Threshold  Converged?
 Maximum Force            0.000772     0.000450     NO
 RMS     Force            0.000274     0.000300     YES
 Maximum Displacement     0.006072     0.001800     NO
 RMS     Displacement     0.002259     0.001200     NO
 Predicted change in Energy=-7.937309D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.662555    1.637865    0.000518
    2          6             0        0.591525    2.439535   -0.000052
    3          1             0        2.716085    1.887314    0.000054
    4          1             0        0.533929    3.520662   -0.001106
    5          6             0       -0.628758    1.582980   -0.000022
```

This journal is © The Royal Society of Chemistry 2014

```
   6          6             0        1.184664    0.225633    0.002676
   7          8             0       -1.785749    1.898273   -0.002428
   8          8             0        1.813269   -0.795584   -0.001578
   9          8             0       -0.209301    0.253326   -0.001685
 ---------------------------------------------------------------------
                   Distance matrix (angstroms):
                    1          2          3          4          5
     1  C    0.000000
     2  C    1.337826   0.000000
     3  H    1.082659   2.195155   0.000000
     4  H    2.195159   1.082661   2.725736   0.000000
     5  C    2.291970   1.490898   3.358659   2.259746   0.000000
     6  C    1.490900   2.291982   2.259743   3.358673   2.265149
     7  O    3.458123   2.438114   4.501848   2.830734   1.199184
     8  O    2.438113   3.458129   2.830727   4.501854   3.408968
     9  O    2.328261   2.328269   3.350791   3.350803   1.394248
                    6          7          8          9
     6  C    0.000000
     7  O    3.408974   0.000000
     8  O    1.199186   4.495530   0.000000
     9  O    1.394247   2.278385   2.278377   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.668909    1.258161   -0.000110
    2          6             0       -0.668918    1.258163   -0.000204
    3          1             0        1.362862    2.089171   -0.001446
    4          1             0       -1.362874    2.089173   -0.001636
    5          6             0       -1.132572   -0.158805    0.001057
    6          6             0        1.132576   -0.158803    0.002949
    7          8             0       -2.247765   -0.599696   -0.000619
    8          8             0        2.247765   -0.599689   -0.001369
    9          8             0        0.000005   -0.971944   -0.000397
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8447627      2.4426831
1.8002372
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
```

```
      nuclear repulsion energy       274.1906192757 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -379.306304596     A.U. after   13 cycles
             Convg  =    0.8269D-08             -V/T =  2.0090
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000447867    0.000469516    0.000399529
    2          6           0.000576446   -0.000300516    0.000110439
    3          1          -0.000000370    0.000023592    0.000014067
    4          1           0.000022797    0.000004676   -0.000029538
    5          6           0.000380110    0.000523635   -0.000393202
    6          6           0.000394811    0.000514001   -0.001197212
    7          8           0.000133212   -0.000424600    0.000133560
    8          8          -0.000443755    0.000007975    0.000425929
    9          8          -0.000615384   -0.000818278    0.000536427
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.001197212 RMS     0.000446160


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000692401 RMS     0.000262924
 Search for a local minimum.
```

This journal is © The Royal Society of Chemistry 2014

```
 Step number   7 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3  5  4
                                                      7  6
 Trust test=-3.94D-01 RLast= 1.89D-02 DXMaxT set to 1.38D-01
 Energy Rises -- skip Quadratic search.
 Quartic linear search produced a step of -0.58232.
 Iteration  1 RMS(Cart)=  0.00131469 RMS(Int)=  0.00000339
 Iteration  2 RMS(Cart)=  0.00000266 RMS(Int)=  0.00000213
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000213
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.52813  -0.00069  -0.00103   0.00000  -0.00103
2.52709
    R2        2.04593   0.00001  -0.00002   0.00000  -0.00002
2.04591
    R3        2.81739   0.00011  -0.00059   0.00000  -0.00059
2.81681
    R4        2.04593   0.00000  -0.00003   0.00000  -0.00003
2.04591
    R5        2.81739   0.00011  -0.00058   0.00000  -0.00058
2.81681
    R6        2.26613  -0.00024  -0.00057   0.00000  -0.00057
2.26556
    R7        2.63475   0.00004   0.00067   0.00000   0.00067
2.63542
    R8        2.26613  -0.00024  -0.00057   0.00000  -0.00057
2.26556
    R9        2.63475   0.00004   0.00068   0.00000   0.00068
2.63543
    A1        2.26656   0.00000  -0.00058   0.00000  -0.00058
2.26598
    A2        1.88704  -0.00005   0.00004   0.00000   0.00004
1.88708
    A3        2.12959   0.00005   0.00054   0.00000   0.00054
2.13013
    A4        2.26656   0.00000  -0.00058   0.00000  -0.00058
2.26598
    A5        1.88703  -0.00005   0.00005   0.00000   0.00005
1.88708
    A6        2.12959   0.00005   0.00053   0.00000   0.00053
2.13013
    A7        2.26352   0.00025   0.00182   0.00000   0.00182
2.26534
    A8        1.87724   0.00036   0.00069   0.00000   0.00070
1.87793
    A9        2.14242  -0.00060  -0.00251   0.00000  -0.00251
2.13991
   A10        2.26351   0.00025   0.00183   0.00000   0.00183
2.26534
```

```
   A11        1.87722   0.00036   0.00070   0.00000   0.00071
1.87793
   A12        2.14241  -0.00060  -0.00251   0.00000  -0.00250
2.13991
   A13        1.89624  -0.00062  -0.00148   0.00000  -0.00148
1.89476
    D1        0.00000   0.00002  -0.00008   0.00000  -0.00008  -
0.00008
    D2        3.14084   0.00008   0.00019   0.00000   0.00018
3.14102
    D3        3.14112   0.00005   0.00008   0.00000   0.00008
3.14120
    D4       -0.00122   0.00011   0.00034   0.00000   0.00034  -
0.00088
    D5        3.13581   0.00027   0.00336   0.00000   0.00335
3.13916
    D6        0.00376  -0.00024  -0.00268   0.00000  -0.00268
0.00109
    D7       -0.00621   0.00030   0.00350   0.00000   0.00349  -
0.00272
    D8       -3.13825  -0.00022  -0.00254   0.00000  -0.00254  -
3.14079
    D9       -3.13942  -0.00015  -0.00276   0.00000  -0.00276
3.14100
   D10       -0.00171   0.00007   0.00211   0.00000   0.00211
0.00039
   D11        0.00149  -0.00010  -0.00253   0.00000  -0.00252  -
0.00104
   D12        3.13920   0.00012   0.00234   0.00000   0.00234
3.14154
   D13        0.00410  -0.00022  -0.00379   0.00000  -0.00380
0.00031
   D14       -3.14104  -0.00002   0.00065   0.00000   0.00065  -
3.14039
   D15       -0.00482   0.00029   0.00399   0.00000   0.00400  -
0.00082
   D16       -3.13768  -0.00019  -0.00152   0.00000  -0.00153  -
3.13921
         Item               Value     Threshold  Converged?
 Maximum Force            0.000692     0.000450     NO
 RMS     Force            0.000263     0.000300     YES
 Maximum Displacement     0.003532     0.001800     NO
 RMS     Displacement     0.001316     0.001200     NO
 Predicted change in Energy=-3.312483D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
```

This journal is © The Royal Society of Chemistry 2014

```
---------------------------------------------------------------------
   1          6             0        1.662502    1.638248    0.000270
   2          6             0        0.591908    2.439586   -0.000363
   3          1             0        2.715875    1.888304    0.000597
   4          1             0        0.534936    3.520733   -0.000627
   5          6             0       -0.628162    1.583261   -0.001387
   6          6             0        1.184768    0.226290    0.000935
   7          8             0       -1.785424    1.896421   -0.001620
   8          8             0        1.811400   -0.795794   -0.000639
   9          8             0       -0.209584    0.252955   -0.000790
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                    1          2          3          4          5
    1  C    0.000000
    2  C    1.337279   0.000000
    3  H    1.082647   2.194345   0.000000
    4  H    2.194346   1.082647   2.724210   0.000000
    5  C    2.291324   1.490592   3.357922   2.259777   0.000000
    6  C    1.490589   2.291324   2.259775   3.357922   2.264529
    7  O    3.457579   2.438593   4.501307   2.832395   1.198885
    8  O    2.438592   3.457577   2.832395   4.501306   3.407545
    9  O    2.328894   2.328894   3.351520   3.351520   1.394605
                    6          7          8          9
    6  C    0.000000
    7  O    3.407548   0.000000
    8  O    1.198885   4.492790   0.000000
    9  O    1.394608   2.276896   2.276895   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
   1          6             0        0.668640    1.258688    0.000078
   2          6             0       -0.668639    1.258689   -0.000077
   3          1             0        1.362106    2.090090   -0.000178
   4          1             0       -1.362104    2.090091   -0.000428
   5          6             0       -1.132264   -0.157967   -0.000365
   6          6             0        1.132265   -0.157965    0.001148
   7          8             0       -2.246396   -0.600724   -0.000021
   8          8             0        2.246394   -0.600726   -0.000646
   9          8             0        0.000000   -0.972156    0.000155
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8374343      2.4453648
1.8011835
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
```

```
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       274.2321197999 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -379.306311035     A.U. after    9 cycles
             Convg  =    0.7019D-08             -V/T =  2.0090
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.000080333    0.000194489    0.000153335
    2          6           0.000162851    0.000130879   -0.000063483
    3          1           0.000026780   -0.000025252    0.000016658
    4          1          -0.000031656    0.000018462   -0.000019764
    5          6           0.000176618   -0.000295763    0.000174136
    6          6          -0.000335152    0.000085278   -0.000457956
    7          8          -0.000310188    0.000180604   -0.000061521
    8          8           0.000261334   -0.000247013    0.000170292
    9          8          -0.000030920   -0.000041685    0.000088303
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000457956 RMS     0.000182429
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000346955 RMS     0.000108097
 Search for a local minimum.
 Step number   8 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3  5  4
                                                      7  6  8
     Eigenvalues ---    0.00476   0.00808   0.01582   0.01665
0.02166
     Eigenvalues ---    0.05548   0.15084   0.16000   0.19397
0.22717
     Eigenvalues ---    0.23749   0.25000   0.28483   0.29892
0.31292
     Eigenvalues ---    0.33394   0.34714   0.34745   0.56033
0.80209
     Eigenvalues ---
0.924361000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.00000
 RFO step:  Lambda=-8.27393182D-06.
 Quartic linear search produced a step of  0.00000.
 Iteration  1 RMS(Cart)=  0.00245911 RMS(Int)=  0.00002189
 Iteration  2 RMS(Cart)=  0.00001315 RMS(Int)=  0.00001715
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00001715
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.52709  -0.00001   0.00000   0.00103   0.00102
2.52812
    R2        2.04591   0.00002   0.00000   0.00006   0.00006
2.04596
    R3        2.81681   0.00019   0.00000   0.00086   0.00086
2.81767
    R4        2.04591   0.00002   0.00000   0.00006   0.00006
2.04597
    R5        2.81681   0.00019   0.00000   0.00085   0.00084
2.81765
    R6        2.26556   0.00035   0.00000   0.00046   0.00046
2.26602
    R7        2.63542   0.00004   0.00000  -0.00079  -0.00079
2.63463
    R8        2.26556   0.00035   0.00000   0.00046   0.00046
2.26603
    R9        2.63543   0.00004   0.00000  -0.00080  -0.00080
2.63463
```

This journal is © The Royal Society of Chemistry 2014

A1	2.26598	0.00004	0.00000	0.00090	0.00089	2.26687
A2	1.88708	-0.00002	0.00000	-0.00018	-0.00017	1.88691
A3	2.13013	-0.00002	0.00000	-0.00072	-0.00072	2.12940
A4	2.26598	0.00004	0.00000	0.00089	0.00089	2.26688
A5	1.88708	-0.00002	0.00000	-0.00018	-0.00018	1.88689
A6	2.13013	-0.00002	0.00000	-0.00072	-0.00071	2.12941
A7	2.26534	-0.00013	0.00000	-0.00231	-0.00231	2.26303
A8	1.87793	0.00004	0.00000	-0.00044	-0.00045	1.87748
A9	2.13991	0.00008	0.00000	0.00276	0.00276	2.14267
A10	2.26534	-0.00013	0.00000	-0.00229	-0.00235	2.26299
A11	1.87793	0.00004	0.00000	-0.00044	-0.00047	1.87746
A12	2.13991	0.00009	0.00000	0.00278	0.00273	2.14263
A13	1.89476	-0.00004	0.00000	0.00124	0.00125	1.89601
D1	-0.00008	0.00002	0.00000	0.00048	0.00048	0.00040
D2	3.14102	0.00005	0.00000	0.00234	0.00233	-3.13983
D3	3.14120	0.00004	0.00000	0.00247	0.00247	-3.13951
D4	-0.00088	0.00008	0.00000	0.00433	0.00432	0.00344
D5	3.13916	0.00009	0.00000	0.01136	0.01134	-3.13269
D6	0.00109	-0.00009	0.00000	-0.00731	-0.00730	-0.00622
D7	-0.00272	0.00012	0.00000	0.01316	0.01315	0.01043
D8	-3.14079	-0.00007	0.00000	-0.00550	-0.00550	3.13690
D9	3.14100	0.00001	0.00000	0.00491	0.00491	-3.13728
D10	0.00039	-0.00004	0.00000	0.00004	0.00005	0.00044
D11	-0.00104	0.00004	0.00000	0.00659	0.00658	0.00555
D12	3.14154	-0.00001	0.00000	0.00172	0.00172	-3.13992
D13	0.00031	-0.00002	0.00000	-0.00471	-0.00471	-0.00441

```
   D14       -3.14039  -0.00006   0.00000  -0.00914  -0.00916
3.13364
   D15       -0.00082   0.00007   0.00000   0.00726   0.00726
0.00644
   D16       -3.13921  -0.00010   0.00000  -0.00976  -0.00980
3.13418
         Item               Value     Threshold  Converged?
 Maximum Force            0.000347     0.000450     YES
 RMS     Force            0.000108     0.000300     YES
 Maximum Displacement     0.010559     0.001800     NO
 RMS     Displacement     0.002460     0.001200     NO
 Predicted change in Energy=-4.141619D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.662594    1.637922   -0.000356
    2          6             0        0.591569    2.439591   -0.000274
    3          1             0        2.716219    1.887042    0.000707
    4          1             0        0.533633    3.520717    0.000543
    5          6             0       -0.628714    1.582793    0.000364
    6          6             0        1.184472    0.225619   -0.004652
    7          8             0       -1.785535    1.898482   -0.003360
    8          8             0        1.813410   -0.795313    0.002176
    9          8             0       -0.209429    0.253150    0.001229
 ---------------------------------------------------------------------
                   Distance matrix (angstroms):
                    1          2          3          4          5
     1  C    0.000000
     2  C    1.337821   0.000000
     3  H    1.082676   2.195324   0.000000
     4  H    2.195329   1.082678   2.726275   0.000000
     5  C    2.291971   1.491037   3.358741   2.259778   0.000000
     6  C    1.491046   2.291991   2.259779   3.358763   2.264860
     7  O    3.457961   2.437915   4.501770   2.830230   1.199128
     8  O    2.437906   3.457962   2.830210   4.501771   3.408718
     9  O    2.328533   2.328545   3.350973   3.350990   1.394185
                    6          7          8          9
     6  C    0.000000
     7  O    3.408726   0.000000
     8  O    1.199130   4.495438   0.000000
     9  O    1.394185   2.278431   2.278410   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
```

This journal is © The Royal Society of Chemistry 2014

```
 Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.668906    1.258187    0.000154
    2          6             0        0.668915    1.258192   -0.000758
    3          1             0       -1.363134    2.088990   -0.000517
    4          1             0        1.363141    2.088999   -0.002044
    5          6             0        1.132424   -0.158971   -0.001617
    6          6             0       -1.132426   -0.158974    0.004804
    7          8             0        2.247720   -0.599441    0.001435
    8          8             0       -2.247717   -0.599430   -0.001311
    9          8             0       -0.000009   -0.972203   -0.001741
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8447683      2.4428376
1.8003249
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       274.1934594689 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
```

```
 SCF Done:  E(RB+HF-LYP) =  -379.306297015     A.U. after   13 cycles
             Convg  =    0.8375D-08             -V/T =  2.0090
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000512937    0.000416310   -0.000672037
    2          6           0.000543629   -0.000379037    0.000216656
    3          1          -0.000016827    0.000030543   -0.000072664
    4          1           0.000034158   -0.000009206    0.000078288
    5          6           0.000469131    0.000665781   -0.000611781
    6          6           0.000506008    0.000642978    0.002037066
    7          8           0.000013362   -0.000454797    0.000267709
    8          8          -0.000436654   -0.000118727   -0.000711557
    9          8          -0.000599870   -0.000793845   -0.000531679
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.002037066 RMS     0.000593398


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000681344 RMS     0.000297642
 Search for a local minimum.
 Step number   9 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3  5  4
                                                    7  6  9  8
 Trust test=-3.39D+00 RLast= 2.78D-02 DXMaxT set to 6.89D-02
 Energy Rises -- skip Quadratic search.
 Quartic linear search produced a step of -0.81447.
 Iteration  1 RMS(Cart)=  0.00200284 RMS(Int)=  0.00000907
 Iteration  2 RMS(Cart)=  0.00000876 RMS(Int)=  0.00000259
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000259
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.52812  -0.00068  -0.00083   0.00000  -0.00083
2.52728
    R2        2.04596  -0.00001  -0.00005   0.00000  -0.00005
2.04592
    R3        2.81767   0.00004  -0.00070   0.00000  -0.00070
2.81696
    R4        2.04597  -0.00001  -0.00005   0.00000  -0.00005
2.04592
    R5        2.81765   0.00004  -0.00069   0.00000  -0.00068
2.81697
    R6        2.26602  -0.00013  -0.00037   0.00000  -0.00037
2.26565
```

This journal is © The Royal Society of Chemistry 2014

R7	2.63463	0.00007	0.00065	0.00000	0.00065
2.63527					
R8	2.26603	-0.00013	-0.00038	0.00000	-0.00038
2.26565					
R9	2.63463	0.00007	0.00065	0.00000	0.00065
2.63528					
A1	2.26687	-0.00003	-0.00073	0.00000	-0.00072
2.26615					
A2	1.88691	-0.00002	0.00014	0.00000	0.00014
1.88705					
A3	2.12940	0.00004	0.00059	0.00000	0.00059
2.12999					
A4	2.26688	-0.00003	-0.00073	0.00000	-0.00073
2.26615					
A5	1.88689	-0.00001	0.00015	0.00000	0.00015
1.88704					
A6	2.12941	0.00004	0.00058	0.00000	0.00058
2.12999					
A7	2.26303	0.00035	0.00189	0.00000	0.00189
2.26491					
A8	1.87748	0.00029	0.00037	0.00000	0.00037
1.87785					
A9	2.14267	-0.00064	-0.00225	0.00000	-0.00225
2.14042					
A10	2.26299	0.00035	0.00191	0.00000	0.00192
2.26492					
A11	1.87746	0.00029	0.00038	0.00000	0.00039
1.87785					
A12	2.14263	-0.00064	-0.00222	0.00000	-0.00221
2.14042					
A13	1.89601	-0.00055	-0.00102	0.00000	-0.00102
1.89499					
D1	0.00040	-0.00007	-0.00039	0.00000	-0.00039
0.00001					
D2	-3.13983	-0.00021	-0.00190	0.00000	-0.00190
3.14146					
D3	-3.13951	-0.00020	-0.00201	0.00000	-0.00201	-
3.14153					
D4	0.00344	-0.00034	-0.00352	0.00000	-0.00352	-
0.00008					
D5	-3.13269	-0.00038	-0.00924	0.00000	-0.00923
3.14127					
D6	-0.00622	0.00043	0.00595	0.00000	0.00595	-
0.00027					
D7	0.01043	-0.00049	-0.01071	0.00000	-0.01070	-
0.00028					
D8	3.13690	0.00032	0.00448	0.00000	0.00448
3.14138					
D9	-3.13728	-0.00003	-0.00400	0.00000	-0.00399	-
3.14127					
D10	0.00044	0.00013	-0.00004	0.00000	-0.00004
0.00040					

```
   D11        0.00555  -0.00016  -0.00536   0.00000  -0.00536
0.00018
   D12       -3.13992   0.00000  -0.00140   0.00000  -0.00140  -
3.14132
   D13       -0.00441   0.00015   0.00384   0.00000   0.00384  -
0.00057
   D14        3.13364   0.00030   0.00746   0.00000   0.00746
3.14110
   D15        0.00644  -0.00035  -0.00591   0.00000  -0.00591
0.00052
   D16        3.13418   0.00041   0.00798   0.00000   0.00798  -
3.14102
         Item               Value     Threshold  Converged?
 Maximum Force            0.000681     0.000450     NO
 RMS     Force            0.000298     0.000300     YES
 Maximum Displacement     0.008601     0.001800     NO
 RMS     Displacement     0.002004     0.001200     NO
 Predicted change in Energy=-7.721064D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.662520    1.638189    0.000154
    2          6             0        0.591845    2.439587   -0.000347
    3          1             0        2.715940    1.888071    0.000619
    4          1             0        0.534694    3.520730   -0.000411
    5          6             0       -0.628265    1.583174   -0.001062
    6          6             0        1.184713    0.226166   -0.000101
    7          8             0       -1.785446    1.896805   -0.001942
    8          8             0        1.811775   -0.795709   -0.000118
    9          8             0       -0.209558    0.252990   -0.000415
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1          2          3          4          5
     1  C    0.000000
     2  C    1.337380   0.000000
     3  H    1.082652   2.194527   0.000000
     4  H    2.194528   1.082653   2.724594   0.000000
     5  C    2.291446   1.490675   3.358076   2.259778   0.000000
     6  C    1.490673   2.291446   2.259776   3.358077   2.264589
     7  O    3.457652   2.438468   4.501395   2.831993   1.198930
     8  O    2.438469   3.457653   2.831994   4.501397   3.407767
     9  O    2.328830   2.328831   3.351422   3.351423   1.394527
                       6          7          8          9
     6  C    0.000000
     7  O    3.407768   0.000000
     8  O    1.198930   4.493288   0.000000
```

```
    9  O    1.394529   2.277181   2.277181   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.668689    1.258597    0.000035
    2          6             0       -0.668691    1.258597    0.000078
    3          1             0        1.362295    2.089889   -0.000047
    4          1             0       -1.362298    2.089888    0.000030
    5          6             0       -1.132294   -0.158154    0.000003
    6          6             0        1.132295   -0.158152    0.000044
    7          8             0       -2.246644   -0.600486   -0.000283
    8          8             0        2.246644   -0.600486   -0.000284
    9          8             0        0.000000   -0.972166    0.000449
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8387897      2.4448914
1.8010204
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       274.2248147128 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -379.306311802     A.U. after   13 cycles
             Convg  =    0.8518D-08             -V/T =  2.0090
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000030734    0.000235082    0.000000475
    2          6           0.000233714    0.000035834   -0.000011524
    3          1           0.000018612   -0.000014944    0.000000040
    4          1          -0.000019526    0.000013313   -0.000001564
    5          6           0.000230384   -0.000117200    0.000028712
    6          6          -0.000178554    0.000187111    0.000004631
    7          8          -0.000249336    0.000062492   -0.000000675
    8          8           0.000130396   -0.000221006    0.000006978
    9          8          -0.000134954   -0.000180683   -0.000027072
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000249336 RMS     0.000126417


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000257002 RMS     0.000081658
 Search for a local minimum.
 Step number  10 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3  5  4
                                                     7  6  9  8 10
     Eigenvalues ---    0.00493   0.01110   0.01654   0.02114
0.05468
     Eigenvalues ---    0.05828   0.15068   0.16000   0.20312
0.22717
     Eigenvalues ---    0.23534   0.25000   0.28483   0.31205
0.31292
     Eigenvalues ---    0.33329   0.34714   0.34746   0.57656
0.80209
     Eigenvalues ---
0.918601000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.00000
 RFO step:  Lambda=-5.45702023D-07.
```

This journal is © The Royal Society of Chemistry 2014

```
 Quartic linear search produced a step of  0.00002.
 Iteration  1 RMS(Cart)=  0.00047351 RMS(Int)=  0.00000027
 Iteration  2 RMS(Cart)=  0.00000032 RMS(Int)=  0.00000008
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.52728  -0.00014   0.00000  -0.00018  -0.00018
2.52711
    R2        2.04592   0.00001   0.00000   0.00004   0.00004
2.04596
    R3        2.81696   0.00016   0.00000   0.00045   0.00045
2.81742
    R4        2.04592   0.00001   0.00000   0.00004   0.00004
2.04596
    R5        2.81697   0.00016   0.00000   0.00045   0.00045
2.81742
    R6        2.26565   0.00026   0.00000   0.00028   0.00028
2.26593
    R7        2.63527   0.00005   0.00000   0.00013   0.00013
2.63540
    R8        2.26565   0.00026   0.00000   0.00028   0.00028
2.26593
    R9        2.63528   0.00005   0.00000   0.00013   0.00013
2.63541
    A1        2.26615   0.00003   0.00000   0.00021   0.00021
2.26636
    A2        1.88705  -0.00002   0.00000  -0.00011  -0.00011
1.88694
    A3        2.12999  -0.00001   0.00000  -0.00011  -0.00011
2.12988
    A4        2.26615   0.00003   0.00000   0.00021   0.00021
2.26636
    A5        1.88704  -0.00002   0.00000  -0.00010  -0.00010
1.88694
    A6        2.12999  -0.00001   0.00000  -0.00011  -0.00011
2.12988
    A7        2.26491  -0.00004   0.00000  -0.00024  -0.00024
2.26467
    A8        1.87785   0.00009   0.00000   0.00032   0.00032
1.87817
    A9        2.14042  -0.00005   0.00000  -0.00008  -0.00008
2.14034
   A10        2.26492  -0.00004   0.00000  -0.00024  -0.00024
2.26467
   A11        1.87785   0.00009   0.00000   0.00032   0.00032
1.87817
   A12        2.14042  -0.00005   0.00000  -0.00008  -0.00008
2.14034
   A13        1.89499  -0.00014   0.00000  -0.00043  -0.00043
1.89455
    D1        0.00001   0.00000   0.00000  -0.00002  -0.00002
0.00000
```

```
    D2        3.14146   0.00000   0.00000   0.00027   0.00027  -
3.14146
    D3       -3.14153   0.00000   0.00000  -0.00021  -0.00021
3.14145
    D4       -0.00008   0.00000   0.00000   0.00008   0.00008
0.00000
    D5        3.14127   0.00000   0.00000   0.00086   0.00086  -
3.14106
    D6       -0.00027   0.00000   0.00000   0.00061   0.00061
0.00034
    D7       -0.00028   0.00000   0.00000   0.00069   0.00069
0.00041
    D8        3.14138   0.00000   0.00000   0.00043   0.00043  -
3.14138
    D9       -3.14127   0.00000   0.00000  -0.00090  -0.00090
3.14101
   D10        0.00040  -0.00001   0.00000  -0.00074  -0.00074  -
0.00034
   D11        0.00018   0.00000   0.00000  -0.00064  -0.00064  -
0.00046
   D12       -3.14132  -0.00001   0.00000  -0.00048  -0.00048
3.14138
   D13       -0.00057   0.00001   0.00000   0.00112   0.00112
0.00055
   D14        3.14110   0.00000   0.00000   0.00127   0.00127  -
3.14081
   D15        0.00052  -0.00001   0.00000  -0.00107  -0.00107  -
0.00055
   D16       -3.14102  -0.00001   0.00000  -0.00131  -0.00131
3.14086
         Item               Value     Threshold  Converged?
 Maximum Force            0.000257     0.000450     YES
 RMS     Force            0.000082     0.000300     YES
 Maximum Displacement     0.001885     0.001800     NO
 RMS     Displacement     0.000474     0.001200     YES
 Predicted change in Energy=-2.728477D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.662598    1.638370    0.000037
    2          6             0        0.591997    2.439712   -0.000508
    3          1             0        2.716094    1.888033    0.000704
    4          1             0        0.534614    3.520866   -0.000404
    5          6             0       -0.628217    1.583035   -0.001158
    6          6             0        1.184566    0.226172   -0.000235
    7          8             0       -1.785500    1.896864   -0.001215
```

```
   8          8             0        1.811847   -0.795743    0.000568
   9          8             0       -0.209778    0.252695   -0.001413
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1          2          3          4          5
    1  C    0.000000
    2  C    1.337287   0.000000
    3  H    1.082675   2.194570   0.000000
    4  H    2.194570   1.082675   2.724885   0.000000
    5  C    2.291484   1.490912   3.358191   2.259948   0.000000
    6  C    1.490912   2.291484   2.259947   3.358191   2.264346
    7  O    3.457774   2.438683   4.501603   2.832015   1.199080
    8  O    2.438684   3.457774   2.832016   4.501603   3.407712
    9  O    2.329354   2.329354   3.351874   3.351874   1.394595
                       6          7          8          9
    6  C    0.000000
    7  O    3.407712   0.000000
    8  O    1.199079   4.493444   0.000000
    9  O    1.394597   2.277321   2.277321   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
   1          6             0        0.668643    1.258814   -0.000063
   2          6             0       -0.668644    1.258814   -0.000074
   3          1             0        1.362442    2.089975    0.000076
   4          1             0       -1.362443    2.089975    0.000056
   5          6             0       -1.132172   -0.158211   -0.000111
   6          6             0        1.132173   -0.158210   -0.000092
   7          8             0       -2.246722   -0.600445    0.000410
   8          8             0        2.246722   -0.600445    0.000399
   9          8             0        0.000000   -0.972509   -0.000572
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8366285      2.4448447
1.8008452
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       274.2052855488 Hartrees.
```

```
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -379.306312043     A.U. after    8 cycles
             Convg  =    0.5383D-08             -V/T =  2.0090
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000037927    0.000045198   -0.000001014
    2          6           0.000053958   -0.000023868   -0.000002345
    3          1           0.000000294   -0.000019609    0.000001429
    4          1          -0.000018884   -0.000005286    0.000001053
    5          6          -0.000008852    0.000008894    0.000009620
    6          6           0.000010434   -0.000006249    0.000003117
    7          8           0.000004844   -0.000009889   -0.000015397
    8          8          -0.000010712    0.000001993   -0.000012755
    9          8           0.000006845    0.000008817    0.000016291
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000053958 RMS     0.000018438


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000032480 RMS     0.000010233
 Search for a local minimum.
 Step number  11 out of a maximum of  48
```

This journal is © The Royal Society of Chemistry 2014

```
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3  5  4
                                                     7  6  9  8 10

                                                    11
 Trust test= 8.83D-01 RLast= 3.31D-03 DXMaxT set to 6.89D-02
     Eigenvalues ---    0.00611   0.01110   0.01661   0.02114
0.05470
     Eigenvalues ---    0.05749   0.13787   0.16000   0.20777
0.22717
     Eigenvalues ---    0.24124   0.25000   0.28483   0.30981
0.31292
     Eigenvalues ---    0.32696   0.34714   0.34780   0.55641
0.80209
     Eigenvalues ---
0.897991000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.00000
 RFO step:  Lambda=-9.21731287D-08.
 Quartic linear search produced a step of -0.10501.
 Iteration  1 RMS(Cart)=  0.00053310 RMS(Int)=  0.00000029
 Iteration  2 RMS(Cart)=  0.00000039 RMS(Int)=  0.00000006
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.52711  -0.00003   0.00002  -0.00010  -0.00008
2.52703
    R2        2.04596   0.00000   0.00000   0.00000   0.00000
2.04596
    R3        2.81742   0.00000  -0.00005   0.00014   0.00009
2.81751
    R4        2.04596   0.00000   0.00000   0.00000   0.00000
2.04596
    R5        2.81742   0.00000  -0.00005   0.00014   0.00009
2.81751
    R6        2.26593  -0.00001  -0.00003   0.00008   0.00005
2.26598
    R7        2.63540  -0.00001  -0.00001  -0.00001  -0.00002
2.63538
    R8        2.26593  -0.00001  -0.00003   0.00008   0.00005
2.26598
    R9        2.63541  -0.00001  -0.00001  -0.00001  -0.00002
2.63538
    A1        2.26636   0.00002  -0.00002   0.00017   0.00015
2.26651
    A2        1.88694   0.00000   0.00001  -0.00003  -0.00002
1.88692
    A3        2.12988  -0.00002   0.00001  -0.00014  -0.00013
2.12976
```

```
    A4        2.26636   0.00002  -0.00002   0.00017   0.00015
2.26651
    A5        1.88694   0.00000   0.00001  -0.00003  -0.00002
1.88692
    A6        2.12988  -0.00002   0.00001  -0.00014  -0.00013
2.12976
    A7        2.26467   0.00001   0.00003  -0.00003  -0.00001
2.26466
    A8        1.87817   0.00000  -0.00003   0.00007   0.00004
1.87821
    A9        2.14034  -0.00001   0.00001  -0.00004  -0.00003
2.14031
   A10        2.26467   0.00001   0.00003  -0.00004  -0.00001
2.26466
   A11        1.87817   0.00000  -0.00003   0.00008   0.00004
1.87821
   A12        2.14034  -0.00001   0.00001  -0.00004  -0.00003
2.14031
   A13        1.89455   0.00000   0.00005  -0.00009  -0.00005
1.89450
    D1        0.00000   0.00000   0.00000   0.00000   0.00001
0.00000
    D2       -3.14146   0.00000  -0.00003  -0.00023  -0.00026
3.14147
    D3        3.14145   0.00000   0.00002   0.00029   0.00031  -
3.14142
    D4        0.00000   0.00000  -0.00001   0.00005   0.00005
0.00005
    D5       -3.14106  -0.00001  -0.00009  -0.00098  -0.00107
3.14106
    D6        0.00034   0.00000  -0.00006  -0.00069  -0.00075  -
0.00041
    D7        0.00041   0.00000  -0.00007  -0.00072  -0.00080  -
0.00038
    D8       -3.14138   0.00000  -0.00005  -0.00043  -0.00048
3.14133
    D9        3.14101   0.00001   0.00010   0.00115   0.00125  -
3.14093
   D10       -0.00034   0.00000   0.00008   0.00060   0.00067
0.00033
   D11       -0.00046   0.00001   0.00007   0.00094   0.00101
0.00055
   D12        3.14138   0.00000   0.00005   0.00038   0.00043  -
3.14137
   D13        0.00055  -0.00001  -0.00012  -0.00103  -0.00115  -
0.00059
   D14       -3.14081  -0.00001  -0.00013  -0.00154  -0.00167
3.14070
   D15       -0.00055   0.00001   0.00011   0.00106   0.00117
0.00062
   D16        3.14086   0.00001   0.00014   0.00133   0.00147  -
3.14086
```

```
         Item               Value     Threshold  Converged?
 Maximum Force            0.000032     0.000450     YES
 RMS     Force            0.000010     0.000300     YES
 Maximum Displacement     0.002175     0.001800     NO
 RMS     Displacement     0.000533     0.001200     YES
 Predicted change in Energy=-4.943149D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.662616    1.638429    0.000208
    2          6             0        0.592049    2.439747   -0.000329
    3          1             0        2.716146    1.887939    0.000625
    4          1             0        0.534509    3.520889   -0.000470
    5          6             0       -0.628191    1.583022   -0.000925
    6          6             0        1.184545    0.226194   -0.000081
    7          8             0       -1.785501    1.896850   -0.002111
    8          8             0        1.811834   -0.795748   -0.000277
    9          8             0       -0.209788    0.252682   -0.000262
 ---------------------------------------------------------------------
                    Distance matrix (angstroms):
                    1          2          3          4          5
     1  C    0.000000
     2  C    1.337245   0.000000
     3  H    1.082673   2.194603   0.000000
     4  H    2.194603   1.082673   2.725082   0.000000
     5  C    2.291477   1.490960   3.358209   2.259911   0.000000
     6  C    1.490960   2.291477   2.259911   3.358209   2.264287
     7  O    3.457789   2.438747   4.501658   2.831952   1.199107
     8  O    2.438747   3.457788   2.831953   4.501657   3.407678
     9  O    2.329419   2.329419   3.351889   3.351888   1.394584
                    6          7          8          9
     6  C    0.000000
     7  O    3.407678   0.000000
     8  O    1.199107   4.493429   0.000000
     9  O    1.394585   2.277315   2.277315   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
```

```
    1          6             0       -0.668622    1.258866   -0.000073
    2          6             0        0.668622    1.258866   -0.000074
    3          1             0       -1.362541    2.089924    0.000068
    4          1             0        1.362541    2.089924    0.000066
    5          6             0        1.132143   -0.158212   -0.000140
    6          6             0       -1.132144   -0.158212   -0.000073
    7          8             0        2.246715   -0.600465    0.000450
    8          8             0       -2.246715   -0.600465    0.000424
    9          8             0        0.000000   -0.972532   -0.000620
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8362416      2.4448775
1.8008361
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   137 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   137 basis functions,   232 primitive gaussians,   137 cartesian
basis functions
    25 alpha electrons       25 beta electrons
       nuclear repulsion energy       274.2035778970 Hartrees.
 NAtoms=    9 NActive=    9 NUniq=    9 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   137 RedAO= T  NBF=   137
 NBsUse=   137 1.00D-06 NBFU=   137
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -379.306312041     A.U. after   13 cycles
             Convg  =    0.5512D-08             -V/T =  2.0090
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
```

This journal is © The Royal Society of Chemistry 2014

```
 Number     Number              X              Y              Z
 ----------------------------------------------------------------------
    1          6          -0.000012762   -0.000015445   -0.000003655
    2          6          -0.000011205   -0.000016590    0.000006677
    3          1          -0.000000626   -0.000009067   -0.000002270
    4          1          -0.000008529   -0.000003106   -0.000000593
    5          6          -0.000050865    0.000029711   -0.000019978
    6          6           0.000042559   -0.000040392    0.000008830
    7          8           0.000051797   -0.000016022    0.000020017
    8          8          -0.000029861    0.000045090    0.000009574
    9          8           0.000019492    0.000025821   -0.000018602
 ----------------------------------------------------------------------
 Cartesian Forces:  Max     0.000051797 RMS     0.000024472


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000054205 RMS     0.000015723
 Search for a local minimum.
 Step number  12 out of a maximum of  48
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3  5  4
                                                     7  6  9  8 10

                                                    12 11
 Trust test=-3.60D-02 RLast= 3.70D-03 DXMaxT set to 5.00D-02
     Eigenvalues ---    0.01110   0.01214   0.01753   0.02114
0.05504
     Eigenvalues ---    0.05824   0.12797   0.16000   0.20386
0.22717
     Eigenvalues ---    0.23378   0.25000   0.28483   0.31172
0.31292
     Eigenvalues ---    0.32818   0.34714   0.34741   0.55928
0.80209
     Eigenvalues ---
0.929481000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.000001000.00000
 RFO step:  Lambda=-1.04920558D-08.
 Quartic linear search produced a step of -0.50873.
 Iteration  1 RMS(Cart)=  0.00027120 RMS(Int)=  0.00000008
 Iteration  2 RMS(Cart)=  0.00000010 RMS(Int)=  0.00000002
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.52703   0.00001   0.00004  -0.00003   0.00001
2.52704
```

This journal is © The Royal Society of Chemistry 2014

R2	2.04596	0.00000	0.00000	-0.00001	-0.00001
2.04595					
R3	2.81751	-0.00002	-0.00005	-0.00002	-0.00007
2.81744					
R4	2.04596	0.00000	0.00000	-0.00001	-0.00001
2.04595					
R5	2.81751	-0.00002	-0.00005	-0.00002	-0.00007
2.81744					
R6	2.26598	-0.00005	-0.00003	-0.00003	-0.00005
2.26593					
R7	2.63538	-0.00001	0.00001	-0.00003	-0.00002
2.63536					
R8	2.26598	-0.00005	-0.00003	-0.00003	-0.00005
2.26593					
R9	2.63538	-0.00001	0.00001	-0.00003	-0.00002
2.63536					
A1	2.26651	0.00001	-0.00007	0.00009	0.00001
2.26652					
A2	1.88692	0.00000	0.00001	0.00001	0.00002
1.88694					
A3	2.12976	-0.00001	0.00007	-0.00010	-0.00003
2.12972					
A4	2.26651	0.00001	-0.00007	0.00009	0.00001
2.26652					
A5	1.88692	0.00000	0.00001	0.00001	0.00002
1.88694					
A6	2.12976	-0.00001	0.00007	-0.00010	-0.00003
2.12972					
A7	2.26466	0.00001	0.00000	0.00004	0.00004
2.26470					
A8	1.87821	-0.00001	-0.00002	-0.00003	-0.00005
1.87816					
A9	2.14031	0.00000	0.00002	-0.00001	0.00001
2.14032					
A10	2.26466	0.00001	0.00000	0.00004	0.00004
2.26470					
A11	1.87821	-0.00001	-0.00002	-0.00003	-0.00005
1.87816					
A12	2.14031	0.00000	0.00002	-0.00001	0.00001
2.14032					
A13	1.89450	0.00002	0.00003	0.00004	0.00007
1.89457					
D1	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D2	3.14147	0.00000	0.00013	-0.00001	0.00012
3.14159					
D3	-3.14142	-0.00001	-0.00016	-0.00001	-0.00017	-
3.14159					
D4	0.00005	0.00000	-0.00002	-0.00002	-0.00004
0.00000					
D5	3.14106	0.00001	0.00055	-0.00001	0.00053
3.14159					

This journal is © The Royal Society of Chemistry 2014

```
    D6       -0.00041   0.00001   0.00038   0.00002   0.00040  -
0.00001
    D7       -0.00038   0.00000   0.00040  -0.00002   0.00038
0.00000
    D8        3.14133   0.00000   0.00024   0.00001   0.00025
3.14159
    D9       -3.14093  -0.00001  -0.00064   0.00000  -0.00064  -
3.14157
   D10        0.00033   0.00000  -0.00034   0.00002  -0.00033
0.00001
   D11        0.00055  -0.00001  -0.00051  -0.00002  -0.00053
0.00002
   D12       -3.14137   0.00000  -0.00022   0.00000  -0.00022  -
3.14159
   D13       -0.00059   0.00001   0.00058   0.00000   0.00058  -
0.00001
   D14        3.14070   0.00002   0.00085   0.00002   0.00087
3.14157
   D15        0.00062  -0.00001  -0.00060  -0.00001  -0.00061
0.00001
   D16       -3.14086  -0.00001  -0.00075   0.00002  -0.00073  -
3.14158
         Item               Value     Threshold  Converged?
 Maximum Force            0.000054     0.000450     YES
 RMS     Force            0.000016     0.000300     YES
 Maximum Displacement     0.001108     0.001800     YES
 RMS     Displacement     0.000271     0.001200     YES
 Predicted change in Energy=-3.133710D-08
 Optimization completed.
    -- Stationary point found.
                           ----------------------------
                           !   Optimized Parameters   !
                           ! (Angstroms and Degrees)  !
 --------------------------                            ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ---------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.3372         -DE/DX =    0.0
!
 ! R2    R(1,3)                  1.0827         -DE/DX =    0.0
!
 ! R3    R(1,6)                  1.491          -DE/DX =    0.0
!
 ! R4    R(2,4)                  1.0827         -DE/DX =    0.0
!
 ! R5    R(2,5)                  1.491          -DE/DX =    0.0
!
 ! R6    R(5,7)                  1.1991         -DE/DX =   -0.0001
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R7    R(5,9)                  1.3946         -DE/DX =    0.0
!
 ! R8    R(6,8)                  1.1991         -DE/DX =   -0.0001
!
 ! R9    R(6,9)                  1.3946         -DE/DX =    0.0
!
 ! A1    A(2,1,3)              129.8613         -DE/DX =    0.0
!
 ! A2    A(2,1,6)              108.1127         -DE/DX =    0.0
!
 ! A3    A(3,1,6)              122.026          -DE/DX =    0.0
!
 ! A4    A(1,2,4)              129.8613         -DE/DX =    0.0
!
 ! A5    A(1,2,5)              108.1127         -DE/DX =    0.0
!
 ! A6    A(4,2,5)              122.026          -DE/DX =    0.0
!
 ! A7    A(2,5,7)              129.7555         -DE/DX =    0.0
!
 ! A8    A(2,5,9)              107.6137         -DE/DX =    0.0
!
 ! A9    A(7,5,9)              122.6308         -DE/DX =    0.0
!
 ! A10   A(1,6,8)              129.7555         -DE/DX =    0.0
!
 ! A11   A(1,6,9)              107.6137         -DE/DX =    0.0
!
 ! A12   A(8,6,9)              122.6308         -DE/DX =    0.0
!
 ! A13   A(5,9,6)              108.5471         -DE/DX =    0.0
!
 ! D1    D(3,1,2,4)              0.0001         -DE/DX =    0.0
!
 ! D2    D(3,1,2,5)            179.993          -DE/DX =    0.0
!
 ! D3    D(6,1,2,4)           -179.9902         -DE/DX =    0.0
!
 ! D4    D(6,1,2,5)              0.0026         -DE/DX =    0.0
!
 ! D5    D(2,1,6,8)            179.9692         -DE/DX =    0.0
!
 ! D6    D(2,1,6,9)             -0.0236         -DE/DX =    0.0
!
 ! D7    D(3,1,6,8)             -0.0221         -DE/DX =    0.0
!
 ! D8    D(3,1,6,9)            179.9852         -DE/DX =    0.0
!
 ! D9    D(1,2,5,7)           -179.9621         -DE/DX =    0.0
!
 ! D10   D(1,2,5,9)              0.0192         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D11   D(4,2,5,7)             0.0315         -DE/DX =    0.0
!
 ! D12   D(4,2,5,9)          -179.9873         -DE/DX =    0.0
!
 ! D13   D(2,5,9,6)            -0.034          -DE/DX =    0.0
!
 ! D14   D(7,5,9,6)           179.9489         -DE/DX =    0.0
!
 ! D15   D(1,6,9,5)             0.0355         -DE/DX =    0.0
!
 ! D16   D(8,6,9,5)          -179.9579         -DE/DX =    0.0
!
 ---------------------------------------------------------------------
-----------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.662616    1.638429    0.000208
    2          6             0        0.592049    2.439747   -0.000329
    3          1             0        2.716146    1.887939    0.000625
    4          1             0        0.534509    3.520889   -0.000470
    5          6             0       -0.628191    1.583022   -0.000925
    6          6             0        1.184545    0.226194   -0.000081
    7          8             0       -1.785501    1.896850   -0.002111
    8          8             0        1.811834   -0.795748   -0.000277
    9          8             0       -0.209788    0.252682   -0.000262
 ---------------------------------------------------------------------
                   Distance matrix (angstroms):
                    1          2          3          4          5
     1  C    0.000000
     2  C    1.337245   0.000000
     3  H    1.082673   2.194603   0.000000
     4  H    2.194603   1.082673   2.725082   0.000000
     5  C    2.291477   1.490960   3.358209   2.259911   0.000000
     6  C    1.490960   2.291477   2.259911   3.358209   2.264287
     7  O    3.457789   2.438747   4.501658   2.831952   1.199107
     8  O    2.438747   3.457788   2.831953   4.501657   3.407678
     9  O    2.329419   2.329419   3.351889   3.351888   1.394584
                    6          7          8          9
     6  C    0.000000
     7  O    3.407678   0.000000
     8  O    1.199107   4.493429   0.000000
     9  O    1.394585   2.277315   2.277315   0.000000
 Stoichiometry    C4H2O3
 Framework group  C1[X(C4H2O3)]
 Deg. of freedom    21
```

```
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6            0       -0.668622    1.258866   -0.000073
    2          6            0        0.668622    1.258866   -0.000074
    3          1            0       -1.362541    2.089924    0.000068
    4          1            0        1.362541    2.089924    0.000066
    5          6            0        1.132143   -0.158212   -0.000140
    6          6            0       -1.132144   -0.158212   -0.000073
    7          8            0        2.246715   -0.600465    0.000450
    8          8            0       -2.246715   -0.600465    0.000424
    9          8            0        0.000000   -0.972532   -0.000620
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      6.8362416      2.4448775
1.8008361


**********************************************************************

            Population analysis using the SCF density.


**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.24500 -19.19777 -19.19777 -10.36865 -
10.36864
 Alpha  occ. eigenvalues --  -10.27120 -10.27033  -1.16767  -1.10538
-1.06741
 Alpha  occ. eigenvalues --   -0.87124  -0.72360  -0.65640  -0.61842
-0.53700
 Alpha  occ. eigenvalues --   -0.52185  -0.50114  -0.48597  -0.46576
-0.44060
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha  occ. eigenvalues --   -0.43446  -0.36162  -0.34471  -0.34203
-0.31497
 Alpha virt. eigenvalues --   -0.13224  -0.00930   0.00370   0.01804
0.01879
 Alpha virt. eigenvalues --    0.02304   0.04065   0.05565   0.05829
0.06742
 Alpha virt. eigenvalues --    0.07910   0.09680   0.10239   0.11058
0.13332
 Alpha virt. eigenvalues --    0.13351   0.13438   0.13864   0.16580
0.18226
 Alpha virt. eigenvalues --    0.18545   0.20052   0.22857   0.23168
0.23873
 Alpha virt. eigenvalues --    0.25897   0.26505   0.28408   0.28635
0.29313
 Alpha virt. eigenvalues --    0.30126   0.31218   0.31231   0.33717
0.34801
 Alpha virt. eigenvalues --    0.36650   0.41357   0.43919   0.44316
0.56827
 Alpha virt. eigenvalues --    0.59716   0.60935   0.66312   0.67013
0.71034
 Alpha virt. eigenvalues --    0.75199   0.77750   0.78552   0.85252
0.86301
 Alpha virt. eigenvalues --    0.87413   0.95177   1.00205   1.00918
1.05769
 Alpha virt. eigenvalues --    1.11153   1.16358   1.19060   1.20023
1.24377
 Alpha virt. eigenvalues --    1.27512   1.28035   1.28146   1.30009
1.32153
 Alpha virt. eigenvalues --    1.32726   1.32973   1.34921   1.36945
1.41355
 Alpha virt. eigenvalues --    1.47014   1.49605   1.55525   1.61333
1.72241
 Alpha virt. eigenvalues --    1.75497   1.75779   1.76575   1.77503
1.80120
 Alpha virt. eigenvalues --    1.85116   1.90752   1.93933   1.97128
2.01859
 Alpha virt. eigenvalues --    2.03086   2.07419   2.13032   2.21697
2.24344
 Alpha virt. eigenvalues --    2.28973   2.32987   2.47923   2.52291
2.58341
 Alpha virt. eigenvalues --    2.66370   2.67336   2.75425   2.81857
2.84709
 Alpha virt. eigenvalues --    2.96584   3.07289   3.19666   3.19740
3.25885
 Alpha virt. eigenvalues --    4.17104   4.17279   4.20453   4.41026
4.48458
 Alpha virt. eigenvalues --    4.53931   5.03907
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C    5.880358  -0.109425   0.325697  -0.005116   0.222682  -
0.049853
```

This journal is © The Royal Society of Chemistry 2014

```
     2  C   -0.109425   5.880358  -0.005116   0.325697  -0.049853
0.222682
     3  H    0.325697  -0.005116   0.457453  -0.001142   0.001098  -
0.014016
     4  H   -0.005116   0.325697  -0.001142   0.457453  -0.014016
0.001098
     5  C    0.222682  -0.049853   0.001098  -0.014016   5.119125  -
0.172097
     6  C   -0.049853   0.222682  -0.014016   0.001098  -0.172097
5.119125
     7  O   -0.053516  -0.090538  -0.000421  -0.002598   0.366929
0.048154
     8  O   -0.090537  -0.053517  -0.002598  -0.000421   0.048154
0.366928
     9  O   -0.117281  -0.117282   0.005706   0.005706   0.069122
0.069122
               7          8          9
     1  C   -0.053516  -0.090537  -0.117281
     2  C   -0.090538  -0.053517  -0.117282
     3  H   -0.000421  -0.002598   0.005706
     4  H   -0.002598  -0.000421   0.005706
     5  C    0.366929   0.048154   0.069122
     6  C    0.048154   0.366928   0.069122
     7  O    8.262759  -0.000886  -0.069689
     8  O   -0.000886   8.262759  -0.069689
     9  O   -0.069689  -0.069689   8.582278
 Mulliken atomic charges:
               1
     1  C   -0.003007
     2  C   -0.003007
     3  H    0.233339
     4  H    0.233339
     5  C    0.408858
     6  C    0.408858
     7  O   -0.460193
     8  O   -0.460193
     9  O   -0.357992
 Sum of Mulliken charges=   0.00000
 Atomic charges with hydrogens summed into heavy atoms:
               1
     1  C    0.230332
     2  C    0.230332
     3  H    0.000000
     4  H    0.000000
     5  C    0.408858
     6  C    0.408858
     7  O   -0.460193
     8  O   -0.460193
     9  O   -0.357992
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=   615.4656
 Charge=     0.0000 electrons
```

```
 Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=     4.4125    Z=    -0.0011  Tot=     4.4125
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=   -49.1828   YY=   -36.6627   ZZ=   -37.7757
   XY=     0.0000   XZ=    -0.0002   YZ=     0.0004
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=    -7.9757   YY=     4.5444   ZZ=     3.4314
   XY=     0.0000   XZ=    -0.0002   YZ=     0.0004
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=     0.0000  YYY=     6.8024  ZZZ=     0.0010  XYY=     0.0000
  XXY=    12.5183  XXZ=    -0.0104  XZZ=     0.0000  YZZ=    -4.1058
  YYZ=     0.0015  XYZ=     0.0001
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=  -583.5857 YYYY=  -208.3165 ZZZZ=   -36.4146 XXXY=     0.0000
 XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0025 ZZZX=     0.0002
 ZZZY=     0.0005 XXYY=  -114.5823 XXZZ=   -86.4676 YYZZ=   -46.6458
 XXYZ=     0.0056 YYXZ=     0.0000 ZZXY=     0.0000
 N-N= 2.742035778970D+02 E-N=-1.435226905833D+03  KE=
3.759179573318D+02
 1\1\GINC-OPT0608\FOpt\RB3LYP\6-31+G(d)\C4H2O3\UCN0868\18-Oct-
2011\0\\#
  opt b3lyp/6-31+g(d) geom=connectivity\\maleic
anhydride\\0,1\C,1.6626
 162571,1.6384294985,0.0002076046\C,0.5920489497,2.4397465369,-
0.000328

9115\H,2.7161463686,1.8879387217,0.0006245816\H,0.5345087372,3.5208892
 963,-0.000470359\C,-0.6281908311,1.583022398,-
0.0009249034\C,1.1845451
 603,0.2261939007,-0.0000811644\O,-1.7855014998,1.8968496765,-
0.0021105
 015\O,1.8118337031,-0.7957481918,-0.0002774609\O,-
0.2097882749,0.25268
 23632,-0.0002616356\\Version=AM64L-G03RevD.01\State=1-A\HF=-
379.306312
 \RMSD=5.512e-09\RMSF=2.447e-
05\Thermal=0.\Dipole=1.0402815,1.3898248,0
 .0010082\PG=C01 [X(C4H2O3)]\\@


 IF OTHER PEOPLE ARE GOING TO TALK, CONVERSATION IS SIMPLY IMPOSSIBLE.

                                                -- WHISTLER'S PRINCIPLE
 Job cpu time:  0 days  0 hours 17 minutes 41.3 seconds.
 File lengths (MBytes):  RWF=     22 Int=      0 D2E=      0 Chk=
7 Scr=      1
 Normal termination of Gaussian 03 at Tue Oct 18 12:29:54 2011.
```

This journal is © The Royal Society of Chemistry 2014

9-Methyl Anthracene

```
Entering Gaussian System, Link 0=g09
 Initial command:
 /usr/local/g09a01/g09/l1.exe /tmp/pbstmp.8339731/Gau-10645.inp -
scrdir=/tmp/pbstmp.8339731/
 Entering Link 1 = /usr/local/g09a01/g09/l1.exe PID=     10646.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2009, Gaussian, Inc.
                    All Rights Reserved.

 This is part of the Gaussian(R) 09 program.  It is based on
 the Gaussian(R) 03 system (copyright 2003, Gaussian, Inc.),
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,
 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be
 used, copied, transmitted, or stored only in accord with that
 written license.

 The following legend is applicable only to US Government
 contracts under FAR:

                       RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is
 subject to restrictions as set forth in subparagraphs (a)
 and (c) of the Commercial Computer Software - Restricted
 Rights clause in FAR 52.227-19.

 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ---------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

```
Warning -- This program may not be used in any manner that
competes with the business of Gaussian, Inc. or will provide
assistance to any competitor of Gaussian, Inc.  The licensee
of this program is prohibited from giving any competitor of
Gaussian, Inc. access to this program.  By using this program,
the user acknowledges that Gaussian, Inc. is engaged in the
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.
-----------------------------------------------------------------


Cite this work as:
Gaussian 09, Revision A.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

******************************************
Gaussian 09:  AM64L-G09RevA.01  8-May-2009
               16-Oct-2012
******************************************
%nprocshared=4
Will use up to    4 processors via shared memory.
%mem=450MW
%chk=methylanthracene.chk
--------------------------------------
# opt b3lyp/6-31+g(d) geom=connectivity
--------------------------------------
1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15/3(2);
2/9=110/2;
```

```
 99//99;
 2/9=110/2;
 3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
 4/5=5,16=3/1;
 5/5=2,38=5/2;
 7//1,2,3,16;
 1/14=-1,18=20,19=15/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 ----------------
 methylanthracene
 ----------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                    -4.80106  -5.39655  -0.01292
 C                    -3.43644  -5.39655  -0.01292
 C                    -2.70355  -4.16533  -0.01292
 C                    -3.42755  -2.93358  -0.01843
 C                    -4.85979  -2.97507  -0.01973
 C                    -5.52357  -4.16737  -0.01636
 C                    -1.30465  -4.14244  -0.00802
 C                    -2.72717  -1.72242  -0.02016
 C                    -1.32823  -1.69953  -0.01453
 C                    -0.60426  -2.93123  -0.00711
 C                     0.82792  -2.88961   0.
 H                     1.37379  -3.84514   0.0066
 C                     1.49166  -1.69726   0.00104
 C                     0.76918  -0.46814  -0.00713
 C                    -0.59547  -0.46829  -0.0145
 H                    -0.74695  -5.09168  -0.0037
 H                    -5.36694  -6.33983  -0.01051
 H                    -2.86711  -6.33828  -0.00981
 H                    -5.4056   -2.01953  -0.02434
 H                    -6.62297  -4.20353  -0.01779
 H                     2.59107  -1.66135   0.0072
 H                     1.33526   0.47504  -0.00604
 H                    -1.16501   0.47333  -0.02077
 C                    -3.50789  -0.39499  -0.02613
 H                    -3.6947   -0.08655   0.98128
 H                    -2.93266   0.35485  -0.52787
 H                    -4.43875  -0.53098  -0.53593


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Initialization pass.
                           ----------------------------
                           !    Initial Parameters    !
                           ! (Angstroms and Degrees)  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ---------------------------                          ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ---------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.3646         estimate D2E/DX2
!
 ! R2    R(1,6)                  1.4258         estimate D2E/DX2
!
 ! R3    R(1,17)                 1.1            estimate D2E/DX2
!
 ! R4    R(2,3)                  1.4328         estimate D2E/DX2
!
 ! R5    R(2,18)                 1.1005         estimate D2E/DX2
!
 ! R6    R(3,4)                  1.4288         estimate D2E/DX2
!
 ! R7    R(3,7)                  1.3991         estimate D2E/DX2
!
 ! R8    R(4,5)                  1.4328         estimate D2E/DX2
!
 ! R9    R(4,8)                  1.3991         estimate D2E/DX2
!
 ! R10   R(5,6)                  1.3646         estimate D2E/DX2
!
 ! R11   R(5,19)                 1.1005         estimate D2E/DX2
!
 ! R12   R(6,20)                 1.1            estimate D2E/DX2
!
 ! R13   R(7,10)                 1.3991         estimate D2E/DX2
!
 ! R14   R(7,16)                 1.101          estimate D2E/DX2
!
 ! R15   R(8,9)                  1.3991         estimate D2E/DX2
!
 ! R16   R(8,24)                 1.54           estimate D2E/DX2
!
 ! R17   R(9,10)                 1.4287         estimate D2E/DX2
!
 ! R18   R(9,15)                 1.4328         estimate D2E/DX2
!
 ! R19   R(10,11)                1.4328         estimate D2E/DX2
!
 ! R20   R(11,12)                1.1005         estimate D2E/DX2
!
 ! R21   R(11,13)                1.3646         estimate D2E/DX2
!
 ! R22   R(13,14)                1.4258         estimate D2E/DX2
!
 ! R23   R(13,21)                1.1            estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R24   R(14,15)              1.3647         estimate D2E/DX2
!
 ! R25   R(14,22)              1.1            estimate D2E/DX2
!
 ! R26   R(15,23)              1.1005         estimate D2E/DX2
!
 ! R27   R(24,25)              1.07           estimate D2E/DX2
!
 ! R28   R(24,26)              1.07           estimate D2E/DX2
!
 ! R29   R(24,27)              1.07           estimate D2E/DX2
!
 ! A1    A(2,1,6)             120.4466        estimate D2E/DX2
!
 ! A2    A(2,1,17)            120.9594        estimate D2E/DX2
!
 ! A3    A(6,1,17)            118.5939        estimate D2E/DX2
!
 ! A4    A(1,2,3)             120.7635        estimate D2E/DX2
!
 ! A5    A(1,2,18)            121.155         estimate D2E/DX2
!
 ! A6    A(3,2,18)            118.0813        estimate D2E/DX2
!
 ! A7    A(2,3,4)             118.7901        estimate D2E/DX2
!
 ! A8    A(2,3,7)             121.7006        estimate D2E/DX2
!
 ! A9    A(4,3,7)             119.5092        estimate D2E/DX2
!
 ! A10   A(3,4,5)             118.7868        estimate D2E/DX2
!
 ! A11   A(3,4,8)             119.5145        estimate D2E/DX2
!
 ! A12   A(5,4,8)             121.6986        estimate D2E/DX2
!
 ! A13   A(4,5,6)             120.765         estimate D2E/DX2
!
 ! A14   A(4,5,19)            118.0759        estimate D2E/DX2
!
 ! A15   A(6,5,19)            121.1591        estimate D2E/DX2
!
 ! A16   A(1,6,5)             120.4476        estimate D2E/DX2
!
 ! A17   A(1,6,20)            118.5627        estimate D2E/DX2
!
 ! A18   A(5,6,20)            120.9896        estimate D2E/DX2
!
 ! A19   A(3,7,10)            120.9763        estimate D2E/DX2
!
 ! A20   A(3,7,16)            119.4985        estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A21   A(10,7,16)            119.5252         estimate D2E/DX2
!
 ! A22   A(4,8,9)              120.9759         estimate D2E/DX2
!
 ! A23   A(4,8,24)             119.499          estimate D2E/DX2
!
 ! A24   A(9,8,24)             119.5251         estimate D2E/DX2
!
 ! A25   A(8,9,10)             119.5096         estimate D2E/DX2
!
 ! A26   A(8,9,15)             121.6954         estimate D2E/DX2
!
 ! A27   A(10,9,15)            118.7949         estimate D2E/DX2
!
 ! A28   A(7,10,9)             119.5142         estimate D2E/DX2
!
 ! A29   A(7,10,11)            121.7035         estimate D2E/DX2
!
 ! A30   A(9,10,11)            118.7822         estimate D2E/DX2
!
 ! A31   A(10,11,12)           118.0746         estimate D2E/DX2
!
 ! A32   A(10,11,13)           120.7675         estimate D2E/DX2
!
 ! A33   A(12,11,13)           121.1578         estimate D2E/DX2
!
 ! A34   A(11,13,14)           120.4489         estimate D2E/DX2
!
 ! A35   A(11,13,21)           120.9732         estimate D2E/DX2
!
 ! A36   A(14,13,21)           118.5779         estimate D2E/DX2
!
 ! A37   A(13,14,15)           120.4423         estimate D2E/DX2
!
 ! A38   A(13,14,22)           118.5802         estimate D2E/DX2
!
 ! A39   A(15,14,22)           120.9774         estimate D2E/DX2
!
 ! A40   A(9,15,14)            120.7641         estimate D2E/DX2
!
 ! A41   A(9,15,23)            118.0731         estimate D2E/DX2
!
 ! A42   A(14,15,23)           121.1628         estimate D2E/DX2
!
 ! A43   A(8,24,25)            109.4712         estimate D2E/DX2
!
 ! A44   A(8,24,26)            109.4712         estimate D2E/DX2
!
 ! A45   A(8,24,27)            109.4712         estimate D2E/DX2
!
 ! A46   A(25,24,26)           109.4713         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A47   A(25,24,27)           109.4712         estimate D2E/DX2
!
 ! A48   A(26,24,27)           109.4712         estimate D2E/DX2
!
 ! D1    D(6,1,2,3)              0.1607         estimate D2E/DX2
!
 ! D2    D(6,1,2,18)           179.9717         estimate D2E/DX2
!
 ! D3    D(17,1,2,3)          -179.854          estimate D2E/DX2
!
 ! D4    D(17,1,2,18)           -0.0429         estimate D2E/DX2
!
 ! D5    D(2,1,6,5)              0.0013         estimate D2E/DX2
!
 ! D6    D(2,1,6,20)           179.9091         estimate D2E/DX2
!
 ! D7    D(17,1,6,5)          -179.9844         estimate D2E/DX2
!
 ! D8    D(17,1,6,20)           -0.0766         estimate D2E/DX2
!
 ! D9    D(1,2,3,4)             -0.2525         estimate D2E/DX2
!
 ! D10   D(1,2,3,7)            179.7643         estimate D2E/DX2
!
 ! D11   D(18,2,3,4)           179.9308         estimate D2E/DX2
!
 ! D12   D(18,2,3,7)            -0.0524         estimate D2E/DX2
!
 ! D13   D(2,3,4,5)              0.1839         estimate D2E/DX2
!
 ! D14   D(2,3,4,8)           -179.9227         estimate D2E/DX2
!
 ! D15   D(7,3,4,5)           -179.8326         estimate D2E/DX2
!
 ! D16   D(7,3,4,8)              0.0609         estimate D2E/DX2
!
 ! D17   D(2,3,7,10)          -179.9531         estimate D2E/DX2
!
 ! D18   D(2,3,7,16)             -0.021          estimate D2E/DX2
!
 ! D19   D(4,3,7,10)             0.0639         estimate D2E/DX2
!
 ! D20   D(4,3,7,16)           179.996          estimate D2E/DX2
!
 ! D21   D(3,4,5,6)              -0.0283         estimate D2E/DX2
!
 ! D22   D(3,4,5,19)          -179.98           estimate D2E/DX2
!
 ! D23   D(8,4,5,6)           -179.9193         estimate D2E/DX2
!
 ! D24   D(8,4,5,19)             0.129          estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D25   D(3,4,8,9)             -0.0966         estimate D2E/DX2
!
 ! D26   D(3,4,8,24)           179.9991         estimate D2E/DX2
!
 ! D27   D(5,4,8,9)            179.7937         estimate D2E/DX2
!
 ! D28   D(5,4,8,24)            -0.1107         estimate D2E/DX2
!
 ! D29   D(4,5,6,1)             -0.0673         estimate D2E/DX2
!
 ! D30   D(4,5,6,20)          -179.9728         estimate D2E/DX2
!
 ! D31   D(19,5,6,1)           179.8829         estimate D2E/DX2
!
 ! D32   D(19,5,6,20)           -0.0226         estimate D2E/DX2
!
 ! D33   D(3,7,10,9)            -0.1515         estimate D2E/DX2
!
 ! D34   D(3,7,10,11)          179.9003         estimate D2E/DX2
!
 ! D35   D(16,7,10,9)          179.9164         estimate D2E/DX2
!
 ! D36   D(16,7,10,11)          -0.0317         estimate D2E/DX2
!
 ! D37   D(4,8,9,10)             0.0089         estimate D2E/DX2
!
 ! D38   D(4,8,9,15)          -179.9202         estimate D2E/DX2
!
 ! D39   D(24,8,9,10)          179.9133         estimate D2E/DX2
!
 ! D40   D(24,8,9,15)           -0.0159         estimate D2E/DX2
!
 ! D41   D(4,8,24,25)           89.7801         estimate D2E/DX2
!
 ! D42   D(4,8,24,26)         -150.2198         estimate D2E/DX2
!
 ! D43   D(4,8,24,27)          -30.2198         estimate D2E/DX2
!
 ! D44   D(9,8,24,25)          -90.1256         estimate D2E/DX2
!
 ! D45   D(9,8,24,26)           29.8744         estimate D2E/DX2
!
 ! D46   D(9,8,24,27)          149.8744         estimate D2E/DX2
!
 ! D47   D(8,9,10,7)             0.115          estimate D2E/DX2
!
 ! D48   D(8,9,10,11)         -179.9353         estimate D2E/DX2
!
 ! D49   D(15,9,10,7)         -179.9538         estimate D2E/DX2
!
 ! D50   D(15,9,10,11)           -0.0041         estimate D2E/DX2
!
```

```
 ! D51   D(8,9,15,14)          179.9107         estimate D2E/DX2
!
 ! D52   D(8,9,15,23)           -0.1009         estimate D2E/DX2
!
 ! D53   D(10,9,15,14)          -0.0189         estimate D2E/DX2
!
 ! D54   D(10,9,15,23)         179.9695         estimate D2E/DX2
!
 ! D55   D(7,10,11,12)           -0.106         estimate D2E/DX2
!
 ! D56   D(7,10,11,13)        -179.9865         estimate D2E/DX2
!
 ! D57   D(9,10,11,12)         179.9455         estimate D2E/DX2
!
 ! D58   D(9,10,11,13)            0.065         estimate D2E/DX2
!
 ! D59   D(10,11,13,14)         -0.1018         estimate D2E/DX2
!
 ! D60   D(10,11,13,21)         179.9569         estimate D2E/DX2
!
 ! D61   D(12,11,13,14)       -179.9786         estimate D2E/DX2
!
 ! D62   D(12,11,13,21)          0.0801         estimate D2E/DX2
!
 ! D63   D(11,13,14,15)            0.078         estimate D2E/DX2
!
 ! D64   D(11,13,14,22)         179.9999         estimate D2E/DX2
!
 ! D65   D(21,13,14,15)       -179.9793         estimate D2E/DX2
!
 ! D66   D(21,13,14,22)          -0.0574         estimate D2E/DX2
!
 ! D67   D(13,14,15,9)           -0.0166         estimate D2E/DX2
!
 ! D68   D(13,14,15,23)         179.9954         estimate D2E/DX2
!
 ! D69   D(22,14,15,9)         -179.9366         estimate D2E/DX2
!
 ! D70   D(22,14,15,23)          0.0754         estimate D2E/DX2
!
 ---------------------------------------------------------------------
-----------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
 Number of steps in this run= 157 maximum allowed number of steps=
162.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
```

This journal is © The Royal Society of Chemistry 2014

Number	Number	Type	X	Y	Z
1	6	0	-4.801064	-5.396550	-0.012916
2	6	0	-3.436441	-5.396550	-0.012916
3	6	0	-2.703550	-4.165329	-0.012916
4	6	0	-3.427547	-2.933582	-0.018434
5	6	0	-4.859787	-2.975073	-0.019734
6	6	0	-5.523570	-4.167366	-0.016363
7	6	0	-1.304649	-4.142440	-0.008020
8	6	0	-2.727170	-1.722415	-0.020155
9	6	0	-1.328229	-1.699531	-0.014530
10	6	0	-0.604260	-2.931234	-0.007110
11	6	0	0.827922	-2.889610	0.000000
12	1	0	1.373792	-3.845137	0.006601
13	6	0	1.491659	-1.697255	0.001042
14	6	0	0.769176	-0.468140	-0.007130
15	6	0	-0.595467	-0.468285	-0.014497
16	1	0	-0.746946	-5.091677	-0.003701
17	1	0	-5.366936	-6.339828	-0.010512
18	1	0	-2.867115	-6.338284	-0.009810
19	1	0	-5.405600	-2.019527	-0.024338
20	1	0	-6.622968	-4.203531	-0.017794
21	1	0	2.591065	-1.661351	0.007202
22	1	0	1.335256	0.475037	-0.006035
23	1	0	-1.165010	0.473332	-0.020769
24	6	0	-3.507887	-0.394995	-0.026125
25	1	0	-3.694699	-0.086552	0.981280
26	1	0	-2.932660	0.354851	-0.527868
27	1	0	-4.438747	-0.530984	-0.535935

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.364623	0.000000			
3	C	2.432174	1.432841	0.000000		
4	C	2.820069	2.462990	1.428777	0.000000	
5	C	2.422199	2.808827	2.462948	1.432841	0.000000
6	C	1.425805	2.422192	2.820023	2.432188	1.364618
7	C	3.714530	2.473328	1.399097	2.442978	3.741910
8	C	4.219047	3.741976	2.443039	1.399091	2.473299
9	C	5.072330	4.255879	2.823415	2.435166	3.754855
10	C	4.867338	3.754872	2.435168	2.823311	4.255772
11	C	6.162013	4.946686	3.754853	4.255736	5.688385
12	H	6.366797	5.054266	4.089942	4.887168	6.294062
13	C	7.299544	6.162073	4.867377	5.072225	6.478743
14	C	7.437529	6.478925	5.072383	4.867342	6.161988
15	C	6.478800	5.688491	4.255837	3.754781	4.946558
16	H	4.065576	2.706735	2.164834	3.441397	4.625552
17	H	1.099996	2.148625	3.438325	3.919669	3.402773
18	H	2.151054	1.100457	2.179105	3.450530	3.909224
19	H	3.430726	3.909220	3.450460	2.179042	1.100455
20	H	2.177763	3.402539	3.919607	3.438530	2.148935

This journal is © The Royal Society of Chemistry 2014

21	H	8.282251	7.091047	5.856898	6.151660	7.565830
22	H	8.492939	7.566021	6.151829	5.856887	7.090980
23	H	6.904815	6.294043	4.887161	4.089761	5.053996
24	C	5.166047	5.002083	3.855199	2.539870	2.912813
25	H	5.514395	5.408438	4.313609	3.029254	3.271546
26	H	6.069162	5.796342	4.555183	3.364257	3.880775
27	H	4.906991	4.995188	4.061148	2.657595	2.533241

		6	7	8	9	10
6	C	0.000000				
7	C	4.219003	0.000000			
8	C	3.714519	2.807175	0.000000		
9	C	4.867350	2.443031	1.399139	0.000000	
10	C	5.072250	1.399130	2.442982	1.428733	0.000000
11	C	6.478764	2.473359	3.741848	2.462821	1.432804
12	H	6.904923	2.694930	4.617852	3.450361	2.179013
13	C	7.437418	3.714613	4.218957	2.819932	2.432210
14	C	7.299521	4.219151	3.714540	2.432177	2.820134
15	C	6.161932	3.741978	2.473263	1.432797	2.462976
16	H	4.865249	1.100955	3.908131	3.441607	2.165152
17	H	2.178109	4.618517	5.318737	6.151709	5.856757
18	H	3.430697	2.695002	4.618002	4.887353	4.090050
19	H	2.151091	4.617881	2.694862	4.089920	4.887164
20	H	1.099994	5.318679	4.618786	5.856986	6.151723
21	H	8.492819	4.618725	5.318656	3.919540	3.438446
22	H	8.282240	5.318853	4.618690	3.438455	3.919746
23	H	6.366564	4.617901	2.694745	2.178994	3.450463
24	C	4.277133	4.347175	1.540000	2.540248	3.855376
25	H	4.581823	4.810539	2.148263	3.032082	4.315083
26	H	5.236879	4.811059	2.148263	2.656727	4.060910
27	H	3.830153	4.810809	2.148263	3.363434	4.554575

		11	12	13	14	15
11	C	0.000000				
12	H	1.100477	0.000000			
13	C	1.364646	2.151121	0.000000		
14	C	2.422193	3.430723	1.425753	0.000000	
15	C	2.808747	3.909163	2.422128	1.364663	0.000000
16	H	2.707272	2.459979	4.066138	4.865771	4.625885
17	H	7.090866	7.187572	8.282146	8.492856	7.565841
18	H	5.054379	4.919486	6.366960	6.905158	6.294227
19	H	6.294000	7.020966	6.904831	6.366707	5.054090
20	H	7.565875	8.004824	8.492876	8.282334	7.091040
21	H	2.148801	2.500135	1.100009	2.177897	3.402626
22	H	3.402686	4.320364	2.177927	1.100014	2.148865
23	H	3.909167	5.009535	3.430716	2.151193	1.100482
24	C	5.002302	5.977905	5.166438	4.277730	2.913365
25	H	5.410559	6.384870	5.518473	4.587891	3.277580
26	H	4.994712	6.039129	4.905658	3.827802	2.530528
27	H	5.795528	6.712940	6.067804	5.235078	3.878999

		16	17	18	19	20
16	H	0.000000				
17	H	4.785628	0.000000			
18	H	2.459509	2.499822	0.000000		

This journal is © The Royal Society of Chemistry 2014

19	H	5.580465	4.320496	5.009569	0.000000	
20	H	5.942780	2.478192	4.320147	2.500380	0.000000
21	H	4.786395	9.231373	7.187887	8.004745	9.558332
22	H	5.943389	9.558336	8.005078	7.187651	9.231601
23	H	5.580716	8.004713	7.021068	4.919041	7.187653
24	C	5.448130	6.228752	5.977754	2.498084	4.920239
25	H	5.891580	6.548549	6.383675	2.770350	5.149993
26	H	5.892093	7.142275	6.713474	3.465061	5.887053
27	H	5.891739	5.905953	6.039170	1.847241	4.304288

		21	22	23	24	25
21	H	0.000000				
22	H	2.478182	0.000000			
23	H	4.320388	2.500310	0.000000		
24	C	6.229124	4.920710	2.498618	0.000000	
25	H	6.552835	5.156610	2.777931	1.070000	0.000000
26	H	5.904482	4.301379	1.842762	1.070000	1.747303
27	H	7.140797	5.884894	3.462860	1.070000	1.747303

		26	27
26	H	0.000000	
27	H	1.747303	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.649748	-0.958533	0.001817
2	6	0	-2.473339	-1.650077	-0.003190
3	6	0	-1.217578	-0.960079	-0.002300
4	6	0	-1.217508	0.468698	-0.001580
5	6	0	-2.473237	1.158745	0.002254
6	6	0	-3.649688	0.467269	0.004595
7	6	0	-0.000011	-1.649283	-0.002470
8	6	0	0.000058	1.157893	-0.002350
9	6	0	1.217658	0.468661	-0.001792
10	6	0	1.217590	-0.960072	-0.000609
11	6	0	2.473346	-1.650001	0.001367
12	1	0	2.459700	-2.750391	0.003187
13	6	0	3.649796	-0.958467	0.003440
14	6	0	3.649833	0.467285	0.001492
15	6	0	2.473321	1.158746	-0.000868
16	1	0	-0.000271	-2.750238	-0.002957
17	1	0	-4.615599	-1.484954	0.003555
18	1	0	-2.459779	-2.750449	-0.004911
19	1	0	-2.459529	2.259114	0.002431
20	1	0	-4.615783	0.993235	0.007092
21	1	0	4.615773	-1.484683	0.005670

```
     22          1           0        4.615818    0.993498    0.003252
     23          1           0        2.459509    2.259140   -0.002313
     24          6           0       -0.000285    2.697892   -0.001597
     25          1           0       -0.003318    3.054064    1.007379
     26          1           0        0.874761    3.054999   -0.503265
     27          1           0       -0.872535    3.054613   -0.508381
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.4133943      0.4522242
0.3433221
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       882.9326386283 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.854539466     A.U. after   14 cycles
            Convg  =    0.4111D-08             -V/T =  2.0096


**********************************************************************

           Population analysis using the SCF density.


**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -10.20491 -10.20385 -10.20383 -10.20131 -
10.20126
 Alpha  occ. eigenvalues --  -10.19942 -10.19942 -10.19917 -10.19917 -
10.19854
 Alpha  occ. eigenvalues --  -10.19854 -10.19780 -10.19780 -10.19590 -
10.18334
 Alpha  occ. eigenvalues --   -0.89065  -0.85643  -0.81173  -0.79899
-0.75700
 Alpha  occ. eigenvalues --   -0.74472  -0.72813  -0.68911  -0.64757
-0.62170
 Alpha  occ. eigenvalues --   -0.59683  -0.58298  -0.54077  -0.53149
-0.50264
 Alpha  occ. eigenvalues --   -0.46846  -0.46778  -0.45736  -0.44206
-0.44064
 Alpha  occ. eigenvalues --   -0.43521  -0.41301  -0.41189  -0.39517
-0.38953
 Alpha  occ. eigenvalues --   -0.38857  -0.38217  -0.36744  -0.35044
-0.33716
 Alpha  occ. eigenvalues --   -0.32492  -0.30892  -0.29578  -0.26274
-0.24718
 Alpha  occ. eigenvalues --   -0.19901
 Alpha virt. eigenvalues --   -0.06923  -0.02129  -0.00759   0.00378
0.01032
 Alpha virt. eigenvalues --    0.01311   0.02024   0.02652   0.02759
0.04582
 Alpha virt. eigenvalues --    0.04773   0.04899   0.04900   0.05624
0.06756
 Alpha virt. eigenvalues --    0.06901   0.07188   0.07297   0.07954
0.09049
 Alpha virt. eigenvalues --    0.09105   0.09370   0.11040   0.11072
0.11797
 Alpha virt. eigenvalues --    0.12448   0.12626   0.13243   0.13551
0.14016
 Alpha virt. eigenvalues --    0.14518   0.14779   0.15814   0.16985
0.17488
 Alpha virt. eigenvalues --    0.17731   0.17955   0.18062   0.18128
0.18543
 Alpha virt. eigenvalues --    0.19178   0.19496   0.19759   0.20244
0.20425
 Alpha virt. eigenvalues --    0.20579   0.20949   0.22290   0.22624
0.23057
 Alpha virt. eigenvalues --    0.23144   0.23593   0.23940   0.24746
0.24788
 Alpha virt. eigenvalues --    0.25126   0.25406   0.25936   0.26285
0.27497
 Alpha virt. eigenvalues --    0.27590   0.27968   0.28021   0.28857
0.29074
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.29573   0.30316   0.30618   0.31029
0.31937
 Alpha virt. eigenvalues --    0.33110   0.34226   0.34453   0.35770
0.35949
 Alpha virt. eigenvalues --    0.36896   0.37778   0.38891   0.39935
0.40456
 Alpha virt. eigenvalues --    0.40752   0.45776   0.47845   0.48941
0.51552
 Alpha virt. eigenvalues --    0.57152   0.59101   0.61111   0.63891
0.64731
 Alpha virt. eigenvalues --    0.65658   0.67256   0.67614   0.68271
0.70520
 Alpha virt. eigenvalues --    0.70693   0.70743   0.72209   0.72357
0.72650
 Alpha virt. eigenvalues --    0.72998   0.73642   0.74124   0.74310
0.75195
 Alpha virt. eigenvalues --    0.75677   0.76942   0.77894   0.78355
0.78503
 Alpha virt. eigenvalues --    0.79891   0.80024   0.80877   0.80929
0.81183
 Alpha virt. eigenvalues --    0.82925   0.84885   0.86655   0.88622
0.89474
 Alpha virt. eigenvalues --    0.90997   0.92106   0.92420   0.93640
0.93977
 Alpha virt. eigenvalues --    0.96131   1.00240   1.01374   1.02532
1.03327
 Alpha virt. eigenvalues --    1.04735   1.06780   1.08732   1.10398
1.10418
 Alpha virt. eigenvalues --    1.11139   1.12989   1.15122   1.15683
1.18386
 Alpha virt. eigenvalues --    1.18852   1.20076   1.20417   1.21807
1.21840
 Alpha virt. eigenvalues --    1.23010   1.24544   1.24682   1.26410
1.27084
 Alpha virt. eigenvalues --    1.32775   1.35989   1.36913   1.37110
1.37448
 Alpha virt. eigenvalues --    1.39583   1.40838   1.44022   1.44110
1.46793
 Alpha virt. eigenvalues --    1.48035   1.48318   1.49229   1.49725
1.50071
 Alpha virt. eigenvalues --    1.54057   1.56222   1.57144   1.58714
1.61718
 Alpha virt. eigenvalues --    1.76051   1.78910   1.79237   1.80178
1.81894
 Alpha virt. eigenvalues --    1.83837   1.85791   1.88588   1.91325
1.92055
 Alpha virt. eigenvalues --    1.92135   1.94094   1.95004   1.96262
1.96320
 Alpha virt. eigenvalues --    1.98309   1.99449   2.03230   2.03498
2.05548
 Alpha virt. eigenvalues --    2.06833   2.08006   2.13850   2.14681
2.17004
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    2.19608   2.21542   2.24000   2.24503
2.26952
 Alpha virt. eigenvalues --    2.28134   2.28257   2.28615   2.30782
2.33025
 Alpha virt. eigenvalues --    2.34775   2.36504   2.37726   2.39646
2.44567
 Alpha virt. eigenvalues --    2.45032   2.46284   2.49914   2.56390
2.58448
 Alpha virt. eigenvalues --    2.63839   2.66156   2.68144   2.68843
2.69503
 Alpha virt. eigenvalues --    2.69937   2.71914   2.74296   2.75806
2.83203
 Alpha virt. eigenvalues --    2.86115   2.87072   2.89621   2.94385
2.96023
 Alpha virt. eigenvalues --    2.96561   3.13925   3.14368   3.30968
3.44617
 Alpha virt. eigenvalues --    3.50403   4.21476   4.24452   4.25404
4.28263
 Alpha virt. eigenvalues --    4.30675   4.32554   4.32674   4.34119
4.39550
 Alpha virt. eigenvalues --    4.42379   4.43235   4.49736   4.52303
4.68272
 Alpha virt. eigenvalues --    4.88077
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C    5.985351   0.234075  -0.458831   0.377709  -0.798892
0.930762
     2  C    0.234075   6.931308  -0.199614  -1.009888   1.507117  -
1.025702
     3  C   -0.458831  -0.199614   7.745316   0.190746   1.139856  -
0.506404
     4  C    0.377709  -1.009888   0.190746   9.574310  -3.556699
1.254133
     5  C   -0.798892   1.507117   1.139856  -3.556699  11.309047  -
2.296246
     6  C    0.930762  -1.025702  -0.506404   1.254133  -2.296246
7.464562
     7  C   -0.033937  -0.092634   0.565047  -1.345198   0.871494  -
0.469086
     8  C    0.013834  -0.287103  -0.235900   1.499532  -1.380370
0.445396
     9  C   -0.031985  -0.084621  -0.968410   0.208096  -0.420388
0.254551
    10  C   -0.018944   0.132226  -1.160456  -0.969122  -0.046769  -
0.075648
    11  C   -0.025389  -0.180056   0.132984  -0.084444  -0.140935
0.030515
    12  H    0.000745   0.004927  -0.010772  -0.000379  -0.000065  -
0.000119
    13  C    0.020481  -0.025375  -0.018768  -0.032140  -0.041317
0.000567
```

This journal is © The Royal Society of Chemistry 2014

14	C	0.000612	0.030500	-0.075461	0.253471	0.115353	-0.035054
15	C	-0.041210	-0.140291	-0.046492	-0.420283	-0.288776	0.115209
16	H	-0.000090	0.005129	-0.050578	0.007887	0.002230	0.001739
17	H	0.289524	-0.005698	0.009626	0.018429	0.005564	-0.008745
18	H	0.025611	0.262495	-0.044339	0.064355	-0.038042	0.015229
19	H	0.009279	-0.029791	0.004015	-0.028734	0.239028	0.027771
20	H	-0.013667	0.016321	0.010304	-0.016168	0.037429	0.267427
21	H	-0.000005	-0.000030	-0.002253	0.000510	-0.000002	-0.000001
22	H	0.000003	0.000002	0.001099	-0.001725	-0.000078	0.000008
23	H	0.000074	0.000008	0.002206	0.013591	0.001949	-0.000249
24	C	-0.057170	0.064615	-0.197556	-0.333502	0.168411	-0.039772
25	H	-0.000140	-0.000723	-0.008209	-0.024902	0.023814	0.014018
26	H	-0.000380	-0.001219	-0.006405	0.005896	-0.003214	-0.001509
27	H	0.002085	-0.000076	-0.027619	-0.013594	0.001806	0.012791

		7	8	9	10	11	12
1	C	-0.033937	0.013834	-0.031985	-0.018944	-0.025389	0.000745
2	C	-0.092634	-0.287103	-0.084621	0.132226	-0.180056	0.004927
3	C	0.565047	-0.235900	-0.968410	-1.160456	0.132984	-0.010772
4	C	-1.345198	1.499532	0.208096	-0.969122	-0.084444	-0.000379
5	C	0.871494	-1.380370	-0.420388	-0.046769	-0.140935	-0.000065
6	C	-0.469086	0.445396	0.254551	-0.075648	0.030515	-0.000119
7	C	7.380079	-0.558231	-1.343285	0.565097	-0.093032	-0.006248
8	C	-0.558231	7.020982	1.497306	-0.236353	-0.288396	0.004650
9	C	-1.343285	1.497306	9.565586	0.195347	-1.011364	0.064392
10	C	0.565097	-0.236353	0.195347	7.742001	-0.198635	-0.044419
11	C	-0.093032	-0.288396	-1.011364	-0.198635	6.932082	0.262523

This journal is © The Royal Society of Chemistry 2014

12	H	-0.006248	0.004650	0.064392	-0.044419	0.262523	0.540687
13	C	-0.034517	0.013699	0.378421	-0.459378	0.234726	0.025661
14	C	-0.467479	0.446666	1.251502	-0.504886	-1.025073	0.015201
15	C	0.869488	-1.379911	-3.549965	1.138617	1.507026	-0.038012
16	H	0.339704	-0.000097	0.007939	-0.050423	0.005083	0.004299
17	H	-0.012804	0.000733	0.000514	-0.002266	-0.000031	0.000000
18	H	-0.006247	0.004650	-0.000372	-0.010753	0.004932	0.000002
19	H	0.000727	0.045553	0.013541	0.002222	0.000014	0.000000
20	H	0.003873	-0.007747	-0.001727	0.001102	0.000002	0.000000
21	H	-0.012771	0.000725	0.018280	0.009660	-0.005693	-0.004303
22	H	0.003878	-0.007760	-0.016246	0.010343	0.016356	-0.000157
23	H	0.000680	0.045917	-0.027564	0.003521	-0.029793	0.000017
24	C	-0.057605	-0.522541	-0.332798	-0.197845	0.064455	-0.000350
25	H	0.000319	-0.082992	-0.024620	-0.008346	-0.000700	0.000000
26	H	-0.000920	-0.098763	-0.013236	-0.027513	-0.000124	0.000000
27	H	-0.000967	-0.098999	0.005737	-0.006377	-0.001241	0.000000

		13	14	15	16	17	18
1	C	0.020481	0.000612	-0.041210	-0.000090	0.289524	0.025611
2	C	-0.025375	0.030500	-0.140291	0.005129	-0.005698	0.262495
3	C	-0.018768	-0.075461	-0.046492	-0.050578	0.009626	-0.044339
4	C	-0.032140	0.253471	-0.420283	0.007887	0.018429	0.064355
5	C	-0.041317	0.115353	-0.288776	0.002230	0.005564	-0.038042
6	C	0.000567	-0.035054	0.115209	0.001739	-0.008745	0.015229
7	C	-0.034517	-0.467479	0.869488	0.339704	-0.012804	-0.006247
8	C	0.013699	0.446666	-1.379911	-0.000097	0.000733	0.004650
9	C	0.378421	1.251502	-3.549965	0.007939	0.000514	-0.000372

This journal is © The Royal Society of Chemistry 2014

10	C	-0.459378	-0.504886	1.138617	-0.050423	-0.002266	-0.010753
11	C	0.234726	-1.025073	1.507026	0.005083	-0.000031	0.004932
12	H	0.025661	0.015201	-0.038012	0.004299	0.000000	0.000002
13	C	5.985377	0.929203	-0.797150	-0.000090	-0.000005	0.000745
14	C	0.929203	7.457856	-2.290287	0.001739	-0.000001	-0.000118
15	C	-0.797150	-2.290287	11.297791	0.002209	-0.000001	-0.000065
16	H	-0.000090	0.001739	0.002209	0.535225	-0.000011	0.004303
17	H	-0.000005	-0.000001	-0.000001	-0.000011	0.533432	-0.004305
18	H	0.000745	-0.000118	-0.000065	0.004303	-0.004305	0.540690
19	H	0.000074	-0.000248	0.001933	0.000001	-0.000166	0.000017
20	H	0.000003	0.000008	-0.000079	0.000000	-0.004099	-0.000157
21	H	0.289542	-0.008839	0.005709	-0.000011	0.000000	0.000000
22	H	-0.013583	0.267619	0.037166	0.000000	0.000000	0.000000
23	H	0.009148	0.027086	0.238777	0.000001	0.000000	0.000000
24	C	-0.057248	-0.040025	0.167853	0.001410	0.000463	-0.000351
25	H	-0.000157	0.013925	0.023514	0.000000	0.000000	0.000000
26	H	0.002051	0.012169	0.001309	0.000000	0.000000	0.000000
27	H	-0.000380	-0.001383	-0.002792	0.000000	0.000000	0.000000

		19	20	21	22	23	24
1	C	0.009279	-0.013667	-0.000005	0.000003	0.000074	-0.057170
2	C	-0.029791	0.016321	-0.000030	0.000002	0.000008	0.064615
3	C	0.004015	0.010304	-0.002253	0.001099	0.002206	-0.197556
4	C	-0.028734	-0.016168	0.000510	-0.001725	0.013591	-0.333502
5	C	0.239028	0.037429	-0.000002	-0.000078	0.001949	0.168411
6	C	0.027771	0.267427	-0.000001	0.000008	-0.000249	-0.039772
7	C	0.000727	0.003873	-0.012771	0.003878	0.000680	-0.057605

This journal is © The Royal Society of Chemistry 2014

8	C	0.045553	-0.007747	0.000725	-0.007760	0.045917	-0.522541
9	C	0.013541	-0.001727	0.018280	-0.016246	-0.027564	-0.332798
10	C	0.002222	0.001102	0.009660	0.010343	0.003521	-0.197845
11	C	0.000014	0.000002	-0.005693	0.016356	-0.029793	0.064455
12	H	0.000000	0.000000	-0.004303	-0.000157	0.000017	-0.000350
13	C	0.000074	0.000003	0.289542	-0.013583	0.009148	-0.057248
14	C	-0.000248	0.000008	-0.008839	0.267619	0.027086	-0.040025
15	C	0.001933	-0.000079	0.005709	0.037166	0.238777	0.167853
16	H	0.000001	0.000000	-0.000011	0.000000	0.000001	0.001410
17	H	-0.000166	-0.004099	0.000000	0.000000	0.000000	0.000463
18	H	0.000017	-0.000157	0.000000	0.000000	0.000000	-0.000351
19	H	0.554684	-0.004363	0.000000	0.000000	-0.000001	-0.013447
20	H	-0.004363	0.533758	0.000000	0.000000	0.000000	-0.001472
21	H	0.000000	0.000000	0.533432	-0.004098	-0.000167	0.000464
22	H	0.000000	0.000000	-0.004098	0.533753	-0.004366	-0.001471
23	H	-0.000001	0.000000	-0.000167	-0.004366	0.554896	-0.013608
24	C	-0.013447	-0.001472	0.000464	-0.001471	-0.013608	6.949720
25	H	-0.000569	0.000000	0.000000	0.000000	-0.000555	0.413420
26	H	0.000125	0.000000	0.000000	0.000010	0.005498	0.465630
27	H	0.005355	0.000010	0.000000	0.000000	0.000121	0.464825

		25	26	27
1	C	-0.000140	-0.000380	0.002085
2	C	-0.000723	-0.001219	-0.000076
3	C	-0.008209	-0.006405	-0.027619
4	C	-0.024902	0.005896	-0.013594
5	C	0.023814	-0.003214	0.001806
6	C	0.014018	-0.001509	0.012791
7	C	0.000319	-0.000920	-0.000967
8	C	-0.082992	-0.098763	-0.098999
9	C	-0.024620	-0.013236	0.005737
10	C	-0.008346	-0.027513	-0.006377
11	C	-0.000700	-0.000124	-0.001241

This journal is © The Royal Society of Chemistry 2014

```
   12  H    0.000000   0.000000   0.000000
   13  C   -0.000157   0.002051  -0.000380
   14  C    0.013925   0.012169  -0.001383
   15  C    0.023514   0.001309  -0.002792
   16  H    0.000000   0.000000   0.000000
   17  H    0.000000   0.000000   0.000000
   18  H    0.000000   0.000000   0.000000
   19  H   -0.000569   0.000125   0.005355
   20  H    0.000000   0.000000   0.000010
   21  H    0.000000   0.000000   0.000000
   22  H    0.000000   0.000010   0.000000
   23  H   -0.000555   0.005498   0.000121
   24  C    0.413420   0.465630   0.464825
   25  H    0.486613  -0.029676  -0.029743
   26  H   -0.029676   0.513171  -0.024839
   27  H   -0.029743  -0.024839   0.513118
Mulliken atomic charges:
             1
    1  C   -0.409503
    2  C   -0.105902
    3  C    0.216868
    4  C    0.368113
    5  C   -0.411305
    6  C   -0.376143
    7  C   -0.065423
    8  C    0.145520
    9  C    0.365369
   10  C    0.217994
   11  C   -0.105791
   12  H    0.181720
   13  C   -0.409588
   14  C   -0.374056
   15  C   -0.411288
   16  H    0.182401
   17  H    0.179851
   18  H    0.181721
   19  H    0.172982
   20  H    0.179242
   21  H    0.179851
   22  H    0.179248
   23  H    0.172811
   24  C   -0.894506
   25  H    0.235710
   26  H    0.201941
   27  H    0.202162
Sum of Mulliken atomic charges =   0.00000
Mulliken charges with hydrogens summed into heavy atoms:
             1
    1  C   -0.229652
    2  C    0.075819
    3  C    0.216868
    4  C    0.368113
```

```
     5  C   -0.238323
     6  C   -0.196901
     7  C    0.116977
     8  C    0.145520
     9  C    0.365369
    10  C    0.217994
    11  C    0.075929
    13  C   -0.229737
    14  C   -0.194808
    15  C   -0.238477
    24  C   -0.254693
 Sum of Mulliken charges with hydrogens summed into heavy atoms =
0.00000
 Electronic spatial extent (au):  <R**2>=           3138.3477
 Charge=              0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=             -0.0007    Y=              0.3855    Z=
0.0288  Tot=              0.3866
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=            -79.6227   YY=            -78.8532   ZZ=
-95.2440
   XY=              0.0019   XZ=              0.0023   YZ=
0.0451
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=              4.9506   YY=              5.7201   ZZ=
-10.6707
   XY=              0.0019   XZ=              0.0023   YZ=
0.0451
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=             -0.0021  YYY=             -4.2969  ZZZ=
0.5331  XYY=             -0.0043
  XXY=             -1.0257  XXZ=             -0.3590  XZZ=
-0.0052  YZZ=              4.4336
  YYZ=              0.0736  XYZ=             -0.0388
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=          -2902.0880 YYYY=          -1091.1376 ZZZZ=           -
124.0895 XXXY=              0.0433
 XXXZ=             -0.0416 YYYX=              0.0253 YYYZ=
0.2531 ZZZX=              0.0060
 ZZZY=              1.6026 XXYY=           -677.7796 XXZZ=           -
625.9997 YYZZ=           -226.6752
 XXYZ=             -1.8284 YYXZ=              0.0547 ZZXY=
-0.0145
 N-N= 8.829326386283D+02 E-N=-3.104811466749D+03  KE=
5.733287235201D+02
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
```

1	6	-0.009964215	-0.009477309	0.000094624
2	6	0.009375602	-0.006728486	0.000236155
3	6	0.003774386	-0.011454221	-0.000111517
4	6	-0.006395850	0.003413201	0.000316518
5	6	-0.003003330	0.010160295	0.000208495
6	6	-0.012605942	-0.004690486	-0.000004774
7	6	0.004045193	-0.006903358	0.000148994
8	6	-0.013044570	0.022169882	-0.001876265
9	6	0.000016211	0.007287776	0.000206164
10	6	0.008203172	-0.008903274	-0.000061795
11	6	0.001365310	-0.011488947	0.000128717
12	1	-0.003322334	0.007532891	-0.000120346
13	6	0.013161879	0.004105621	0.000085741
14	6	0.010125859	0.008773602	0.000225441
15	6	-0.007345040	0.007577035	0.000261812
16	1	-0.004138666	0.007104173	0.000027310
17	1	0.005574785	0.006395778	-0.000066197
18	1	-0.004947985	0.006563897	-0.000070582
19	1	0.001639571	-0.013640323	0.001061760
20	1	0.008284666	0.001809103	0.000001429
21	1	-0.008305614	-0.001797408	-0.000044627
22	1	-0.005589708	-0.006388774	-0.000111470
23	1	0.011184095	-0.008088691	0.001066511
24	6	0.017380965	-0.029449652	-0.004080475
25	1	-0.005144461	0.008595281	0.016748154
26	1	0.001609124	0.012759084	-0.007078225
27	1	-0.011933103	0.004763311	-0.007191550

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.029449652 RMS     0.008034968


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.020699717 RMS     0.005226677
 Search for a local minimum.
 Step number   1 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- RFO/linear search
 Second derivative matrix not updated -- first step.
     Eigenvalues ---    0.00237   0.01360   0.01759   0.01761
0.01770
     Eigenvalues ---    0.01819   0.01820   0.01929   0.01979
0.01981
     Eigenvalues ---    0.02000   0.02009   0.02100   0.02100
0.02119
     Eigenvalues ---    0.02119   0.02155   0.02155   0.02223
0.02226
     Eigenvalues ---    0.02348   0.02351   0.07243   0.07243
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
```

```
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.22000   0.22000   0.22493
0.22571
     Eigenvalues ---    0.23574   0.24474   0.24551   0.25000
0.25000
     Eigenvalues ---    0.25000   0.28519   0.33577   0.33629
0.33629
     Eigenvalues ---    0.33632   0.33632   0.33681   0.33681
0.33683
     Eigenvalues ---    0.33683   0.35786   0.37230   0.37230
0.37230
     Eigenvalues ---    0.38240   0.38550   0.38614   0.40222
0.40749
     Eigenvalues ---    0.41161   0.41414   0.41942   0.44931
0.45767
     Eigenvalues ---    0.45768   0.49847   0.49859   0.51295
0.51336
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-1.22931128D-02 EMin= 2.36824089D-03
 Linear search not attempted -- first point.
 Iteration  1 RMS(Cart)=  0.06037621 RMS(Int)=  0.00095107
 Iteration  2 RMS(Cart)=  0.00161070 RMS(Int)=  0.00012312
 Iteration  3 RMS(Cart)=  0.00000127 RMS(Int)=  0.00012311
```

This journal is © The Royal Society of Chemistry 2014

```
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00012311
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.57876   0.00299   0.00000   0.00503   0.00496
2.58372
    R2        2.69438   0.00018   0.00000  -0.00021  -0.00025
2.69413
    R3        2.07869  -0.00835   0.00000  -0.02392  -0.02392
2.05477
    R4        2.70768   0.00117   0.00000   0.00267   0.00265
2.71033
    R5        2.07956  -0.00818   0.00000  -0.02346  -0.02346
2.05610
    R6        2.70000   0.01432   0.00000   0.03441   0.03445
2.73444
    R7        2.64391  -0.00131   0.00000  -0.00491  -0.00496
2.63895
    R8        2.70768   0.00729   0.00000   0.01819   0.01825
2.72593
    R9        2.64390   0.02063   0.00000   0.04600   0.04605
2.68995
   R10        2.57875   0.00620   0.00000   0.01172   0.01174
2.59050
   R11        2.07956  -0.01266   0.00000  -0.03632  -0.03632
2.04324
   R12        2.07869  -0.00834   0.00000  -0.02389  -0.02389
2.05480
   R13        2.64397  -0.00134   0.00000  -0.00495  -0.00500
2.63897
   R14        2.08050  -0.00822   0.00000  -0.02362  -0.02362
2.05688
   R15        2.64399   0.02070   0.00000   0.04616   0.04621
2.69020
   R16        2.91018  -0.00384   0.00000  -0.01289  -0.01289
2.89729
   R17        2.69991   0.01441   0.00000   0.03465   0.03469
2.73460
   R18        2.70759   0.00736   0.00000   0.01835   0.01842
2.72601
   R19        2.70761   0.00119   0.00000   0.00274   0.00271
2.71032
   R20        2.07960  -0.00819   0.00000  -0.02349  -0.02349
2.05611
   R21        2.57881   0.00294   0.00000   0.00493   0.00486
2.58367
   R22        2.69428   0.00020   0.00000  -0.00019  -0.00023
2.69406
   R23        2.07872  -0.00836   0.00000  -0.02395  -0.02395
2.05477
   R24        2.57884   0.00617   0.00000   0.01166   0.01169
2.59053
```

This journal is © The Royal Society of Chemistry 2014

R25	2.07873	-0.00835	0.00000	-0.02393	-0.02393
2.05479					
R26	2.07961	-0.01272	0.00000	-0.03648	-0.03648
2.04313					
R27	2.02201	0.01914	0.00000	0.04978	0.04978
2.07178					
R28	2.02201	0.01313	0.00000	0.03413	0.03413
2.05614					
R29	2.02201	0.01320	0.00000	0.03433	0.03433
2.05634					
A1	2.10219	-0.00173	0.00000	-0.01042	-0.01054
2.09165					
A2	2.11114	-0.00069	0.00000	-0.00378	-0.00372
2.10742					
A3	2.06985	0.00241	0.00000	0.01420	0.01426
2.08411					
A4	2.10772	0.00225	0.00000	0.00765	0.00754
2.11526					
A5	2.11455	-0.00200	0.00000	-0.00889	-0.00884
2.10572					
A6	2.06091	-0.00025	0.00000	0.00124	0.00129
2.06220					
A7	2.07328	0.00338	0.00000	0.01526	0.01531
2.08858					
A8	2.12408	-0.00553	0.00000	-0.01950	-0.01945
2.10462					
A9	2.08583	0.00215	0.00000	0.00424	0.00414
2.08997					
A10	2.07322	-0.00939	0.00000	-0.03590	-0.03582
2.03741					
A11	2.08592	-0.00012	0.00000	0.00268	0.00263
2.08855					
A12	2.12404	0.00951	0.00000	0.03320	0.03314
2.15718					
A13	2.10775	0.00408	0.00000	0.01871	0.01877
2.12652					
A14	2.06081	0.00351	0.00000	0.02289	0.02284
2.08365					
A15	2.11463	-0.00760	0.00000	-0.04160	-0.04165
2.07298					
A16	2.10221	0.00141	0.00000	0.00468	0.00465
2.10685					
A17	2.06931	0.00089	0.00000	0.00693	0.00694
2.07625					
A18	2.11167	-0.00230	0.00000	-0.01160	-0.01159
2.10008					
A19	2.11143	0.00404	0.00000	0.00899	0.00881
2.12025					
A20	2.08564	-0.00199	0.00000	-0.00432	-0.00427
2.08137					
A21	2.08611	-0.00205	0.00000	-0.00469	-0.00464
2.08146					

This journal is © The Royal Society of Chemistry 2014

A22	2.11143	-0.00805	0.00000	-0.02277	-0.02274
2.08868					
A23	2.08565	0.00391	0.00000	0.01093	0.01086
2.09651					
A24	2.08611	0.00414	0.00000	0.01181	0.01174
2.09785					
A25	2.08584	-0.00018	0.00000	0.00250	0.00244
2.08828					
A26	2.12399	0.00966	0.00000	0.03373	0.03367
2.15765					
A27	2.07336	-0.00948	0.00000	-0.03624	-0.03616
2.03720					
A28	2.08592	0.00216	0.00000	0.00431	0.00420
2.09012					
A29	2.12413	-0.00559	0.00000	-0.01978	-0.01973
2.10440					
A30	2.07314	0.00343	0.00000	0.01548	0.01552
2.08866					
A31	2.06079	-0.00024	0.00000	0.00132	0.00137
2.06216					
A32	2.10779	0.00224	0.00000	0.00764	0.00753
2.11532					
A33	2.11460	-0.00201	0.00000	-0.00897	-0.00891
2.10569					
A34	2.10223	-0.00174	0.00000	-0.01051	-0.01064
2.09159					
A35	2.11138	-0.00071	0.00000	-0.00394	-0.00389
2.10750					
A36	2.06958	0.00246	0.00000	0.01446	0.01452
2.08409					
A37	2.10211	0.00144	0.00000	0.00480	0.00477
2.10689					
A38	2.06962	0.00084	0.00000	0.00668	0.00669
2.07631					
A39	2.11145	-0.00229	0.00000	-0.01148	-0.01147
2.09999					
A40	2.10773	0.00411	0.00000	0.01883	0.01890
2.12663					
A41	2.06076	0.00355	0.00000	0.02309	0.02304
2.08380					
A42	2.11469	-0.00766	0.00000	-0.04192	-0.04197
2.07272					
A43	1.91063	0.00335	0.00000	0.02234	0.02179
1.93242					
A44	1.91063	0.00652	0.00000	0.03641	0.03593
1.94657					
A45	1.91063	0.00642	0.00000	0.03577	0.03530
1.94593					
A46	1.91063	-0.00432	0.00000	-0.02212	-0.02263
1.88800					
A47	1.91063	-0.00430	0.00000	-0.02211	-0.02261
1.88802					

This journal is © The Royal Society of Chemistry 2014

A48	1.91063	-0.00767	0.00000	-0.05030	-0.05069	1.85994
D1	0.00280	-0.00013	0.00000	-0.00374	-0.00377	-0.00097
D2	3.14110	-0.00020	0.00000	-0.00589	-0.00594	3.13515
D3	-3.13904	0.00004	0.00000	0.00138	0.00136	-3.13769
D4	-0.00075	-0.00004	0.00000	-0.00077	-0.00082	-0.00157
D5	0.00002	0.00017	0.00000	0.00557	0.00559	0.00561
D6	3.14001	0.00025	0.00000	0.00827	0.00831	-3.13487
D7	-3.14132	0.00001	0.00000	0.00057	0.00053	-3.14079
D8	-0.00134	0.00009	0.00000	0.00327	0.00325	0.00191
D9	-0.00441	-0.00016	0.00000	-0.00562	-0.00570	-0.01011
D10	3.13748	-0.00032	0.00000	-0.01066	-0.01075	3.12673
D11	3.14038	-0.00008	0.00000	-0.00352	-0.00356	3.13682
D12	-0.00091	-0.00025	0.00000	-0.00855	-0.00861	-0.00952
D13	0.00321	0.00037	0.00000	0.01290	0.01278	0.01599
D14	-3.14024	0.00011	0.00000	0.00428	0.00439	-3.13586
D15	-3.13867	0.00053	0.00000	0.01782	0.01778	-3.12089
D16	0.00106	0.00027	0.00000	0.00920	0.00939	0.01045
D17	-3.14077	0.00056	0.00000	0.01662	0.01671	-3.12407
D18	-0.00037	0.00006	0.00000	0.00200	0.00199	0.00162
D19	0.00112	0.00039	0.00000	0.01155	0.01165	0.01277
D20	3.14152	-0.00010	0.00000	-0.00307	-0.00306	3.13846
D21	-0.00049	-0.00034	0.00000	-0.01134	-0.01125	-0.01174
D22	-3.14124	-0.00067	0.00000	-0.02135	-0.02142	3.12052
D23	-3.14018	-0.00006	0.00000	-0.00248	-0.00246	3.14055
D24	0.00225	-0.00039	0.00000	-0.01250	-0.01263	-0.01037
D25	-0.00169	-0.00095	0.00000	-0.03079	-0.03058	-0.03227

This journal is © The Royal Society of Chemistry 2014

```
   D26        3.14158  -0.00054   0.00000  -0.01407  -0.01407
3.12751
   D27        3.13799  -0.00124   0.00000  -0.03975  -0.03966
3.09833
   D28       -0.00193  -0.00083   0.00000  -0.02303  -0.02314  -
0.02508
   D29       -0.00117   0.00007   0.00000   0.00215   0.00226
0.00109
   D30       -3.14112  -0.00001   0.00000  -0.00063  -0.00052
3.14155
   D31        3.13955   0.00042   0.00000   0.01250   0.01240  -
3.13123
   D32       -0.00039   0.00034   0.00000   0.00972   0.00962
0.00923
   D33       -0.00265  -0.00038   0.00000  -0.01096  -0.01106  -
0.01371
   D34        3.13985  -0.00055   0.00000  -0.01612  -0.01620
3.12366
   D35        3.14013   0.00012   0.00000   0.00367   0.00366  -
3.13940
   D36       -0.00055  -0.00005   0.00000  -0.00149  -0.00148  -
0.00203
   D37        0.00016   0.00098   0.00000   0.03139   0.03118
0.03134
   D38       -3.14020   0.00128   0.00000   0.04087   0.04078  -
3.09942
   D39        3.14008   0.00056   0.00000   0.01467   0.01465  -
3.12845
   D40       -0.00028   0.00086   0.00000   0.02415   0.02425
0.02398
   D41        1.56696  -0.00022   0.00000  -0.00825  -0.00832
1.55864
   D42       -2.62183   0.00053   0.00000   0.00064   0.00062  -
2.62121
   D43       -0.52744  -0.00094   0.00000  -0.01676  -0.01687  -
0.54430
   D44       -1.57299   0.00020   0.00000   0.00825   0.00831  -
1.56468
   D45        0.52141   0.00095   0.00000   0.01714   0.01725
0.53866
   D46        2.61580  -0.00052   0.00000  -0.00025  -0.00023
2.61557
   D47        0.00201  -0.00031   0.00000  -0.01038  -0.01058  -
0.00857
   D48       -3.14046  -0.00015   0.00000  -0.00539  -0.00550
3.13722
   D49       -3.14079  -0.00059   0.00000  -0.01953  -0.01948
3.12292
   D50       -0.00007  -0.00043   0.00000  -0.01454  -0.01441  -
0.01448
   D51        3.14003   0.00006   0.00000   0.00229   0.00226  -
3.14089
```

```
   D52       -0.00176   0.00038   0.00000   0.01184   0.01196
0.01020
   D53       -0.00033   0.00035   0.00000   0.01168   0.01158
0.01125
   D54        3.14106   0.00067   0.00000   0.02122   0.02128  -
3.12084
   D55       -0.00185   0.00027   0.00000   0.00952   0.00958
0.00773
   D56       -3.14136   0.00038   0.00000   0.01247   0.01257  -
3.12879
   D57        3.14064   0.00011   0.00000   0.00440   0.00446  -
3.13809
   D58        0.00113   0.00021   0.00000   0.00735   0.00744
0.00858
   D59       -0.00178   0.00010   0.00000   0.00315   0.00320
0.00142
   D60        3.14084  -0.00007   0.00000  -0.00242  -0.00238
3.13846
   D61       -3.14122   0.00021   0.00000   0.00618   0.00625  -
3.13497
   D62        0.00140   0.00003   0.00000   0.00061   0.00066
0.00206
   D63        0.00136  -0.00019   0.00000  -0.00634  -0.00636  -
0.00500
   D64        3.14159  -0.00020   0.00000  -0.00701  -0.00705
3.13454
   D65       -3.14123  -0.00002   0.00000  -0.00092  -0.00086
3.14109
   D66       -0.00100  -0.00003   0.00000  -0.00158  -0.00155  -
0.00255
   D67       -0.00029  -0.00004   0.00000  -0.00125  -0.00137  -
0.00166
   D68        3.14151  -0.00037   0.00000  -0.01110  -0.01102
3.13050
   D69       -3.14049  -0.00003   0.00000  -0.00058  -0.00069  -
3.14118
   D70        0.00132  -0.00036   0.00000  -0.01043  -0.01034  -
0.00902
         Item               Value     Threshold  Converged?
 Maximum Force            0.020700     0.000450     NO
 RMS     Force            0.005227     0.000300     NO
 Maximum Displacement     0.236340     0.001800     NO
 RMS     Displacement     0.059968     0.001200     NO
 Predicted change in Energy=-6.463969D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

This journal is © The Royal Society of Chemistry 2014

1	6	0	-4.784344	-5.441070	0.001756
2	6	0	-3.417953	-5.398118	-0.020555
3	6	0	-2.714074	-4.148526	-0.031741
4	6	0	-3.458039	-2.907422	-0.031990
5	6	0	-4.896316	-3.012993	-0.000066
6	6	0	-5.532156	-4.227344	0.015473
7	6	0	-1.317914	-4.119441	-0.036674
8	6	0	-2.759483	-1.667291	-0.050188
9	6	0	-1.336081	-1.659830	-0.028055
10	6	0	-0.613566	-2.913638	-0.026683
11	6	0	0.820558	-2.906630	-0.009840
12	1	0	1.338682	-3.863386	-0.012545
13	6	0	1.522824	-1.733816	0.015055
14	6	0	0.826225	-0.490011	0.026391
15	6	0	-0.544027	-0.454688	0.006702
16	1	0	-0.766335	-5.057783	-0.033474
17	1	0	-5.310470	-6.392566	0.013762
18	1	0	-2.834164	-6.316273	-0.025199
19	1	0	-5.494049	-2.112245	0.020837
20	1	0	-6.618050	-4.278223	0.039579
21	1	0	2.610045	-1.737048	0.030633
22	1	0	1.398834	0.433972	0.052915
23	1	0	-1.039944	0.505843	0.026600
24	6	0	-3.537381	-0.346253	-0.069304
25	1	0	-3.744746	-0.003425	0.951202
26	1	0	-2.983332	0.435979	-0.584103
27	1	0	-4.486171	-0.449787	-0.591972

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.367248	0.000000			
3	C	2.440862	1.434242	0.000000		
4	C	2.859999	2.491045	1.447005	0.000000	
5	C	2.430658	2.806208	2.460207	1.442500	0.000000
6	C	1.425673	2.416995	2.819579	2.458944	1.370833
7	C	3.710029	2.458748	1.396472	2.459502	3.745735
8	C	4.283009	3.788605	2.481719	1.423459	2.525763
9	C	5.117536	4.278907	2.844729	2.461545	3.808819
10	C	4.876895	3.746634	2.436618	2.844485	4.283985
11	C	6.151296	4.916565	3.746520	4.278655	5.717872
12	H	6.323032	4.998104	4.062820	4.891091	6.292736
13	C	7.316028	6.151394	4.876917	5.117476	6.545371
14	C	7.482785	6.488819	5.091349	4.919574	6.254088
15	C	6.545558	5.718191	4.284277	3.809051	5.048504
16	H	4.036403	2.673402	2.149521	3.445189	4.608582
17	H	1.087335	2.138159	3.432063	3.947129	3.404883
18	H	2.137734	1.088044	2.171081	3.465477	3.894196
19	H	3.403693	3.887011	3.446370	2.186420	1.081235
20	H	2.171664	3.390929	3.906781	3.445270	2.136995
21	H	8.270284	7.052858	5.845114	6.180238	7.614094

22	H	8.529386	7.564398	6.158123	5.895875	7.177276
23	H	7.027582	6.365053	4.946642	4.183418	5.220586
24	C	5.245677	5.053512	3.890569	2.562670	2.993827
25	H	5.616956	5.491249	4.382959	3.079296	3.359840
26	H	6.174673	5.877344	4.625505	3.421770	3.986981
27	H	5.035309	5.094467	4.139428	2.722243	2.662442
		6	7	8	9	10
6	C	0.000000				
7	C	4.215946	0.000000			
8	C	3.774373	2.844529	0.000000		
9	C	4.919458	2.459693	1.423594	0.000000	
10	C	5.091181	1.396483	2.481712	1.447088	0.000000
11	C	6.488598	2.458596	3.788705	2.491171	1.434240
12	H	6.880527	2.669016	4.649646	3.465581	2.171058
13	C	7.482675	3.709942	4.283321	2.860187	2.440878
14	C	7.375418	4.215930	3.774806	2.459067	2.819536
15	C	6.254154	3.745824	2.526241	1.442542	2.460160
16	H	4.837879	1.088455	3.932983	3.445391	2.149590
17	H	2.176542	4.594578	5.370274	6.180316	5.845125
18	H	3.412395	2.669311	4.649649	4.891495	4.063125
19	H	2.115450	4.633816	2.771439	4.182794	4.946069
20	H	1.087353	5.303063	4.659781	5.895740	6.157947
21	H	8.514531	4.594473	5.370589	3.947318	3.432101
22	H	8.352718	5.303048	4.660208	3.445334	3.906736
23	H	6.525576	4.634061	2.772223	2.186509	3.446373
24	C	4.364537	4.377676	1.533177	2.563768	3.891269
25	H	4.681016	4.879242	2.177608	3.082903	4.385190
26	H	5.348138	4.881101	2.181495	2.723058	4.140827
27	H	3.966486	4.879813	2.181124	3.421298	4.624629
		11	12	13	14	15
11	C	0.000000				
12	H	1.088045	0.000000			
13	C	1.367219	2.137694	0.000000		
14	C	2.416897	3.412299	1.425633	0.000000	
15	C	2.806133	3.894122	2.430661	1.370849	0.000000
16	H	2.673247	2.420354	4.036255	4.837806	4.608635
17	H	7.052788	7.113977	8.270300	8.514655	7.614292
18	H	4.998290	4.840399	6.323281	6.880875	6.293166
19	H	6.364452	7.053639	7.027072	6.525147	5.220193
20	H	7.564166	7.967709	8.529270	8.352722	7.177344
21	H	2.138182	2.477809	1.087337	2.176495	3.404877
22	H	3.390864	4.298277	2.171662	1.087350	2.136951
23	H	3.886871	4.974892	3.403526	2.115257	1.081179
24	C	5.054770	6.012440	5.247678	4.367022	2.996282
25	H	5.494925	6.455179	5.622981	4.688904	3.367540
26	H	5.096312	6.122991	5.037107	3.967731	2.663184
27	H	5.876762	6.776231	6.174564	5.348416	3.987348
		16	17	18	19	20
16	H	0.000000				
17	H	4.736354	0.000000			
18	H	2.420700	2.477788	0.000000		
19	H	5.570496	4.284262	4.975034	0.000000	

This journal is © The Royal Society of Chemistry 2014

20	H	5.903865	2.486137	4.298329	2.440327	0.000000
21	H	4.736172	9.187420	7.114199	8.112780	9.571593
22	H	5.903795	9.571725	7.968073	7.348203	9.299215
23	H	5.570673	8.113298	7.054302	5.166572	7.348654
24	C	5.466123	6.301480	6.011456	2.637310	4.996276
25	H	5.948702	6.644653	6.452486	2.893572	5.230758
26	H	5.949764	7.238926	6.776986	3.628098	5.985304
27	H	5.948339	6.030175	6.120950	2.038411	4.427267

		21	22	23	24	25
21	H	0.000000				
22	H	2.486133	0.000000			
23	H	4.284040	2.439979	0.000000		
24	C	6.303582	4.998991	2.640540	0.000000	
25	H	6.651035	5.239719	2.903480	1.096341	0.000000
26	H	6.032066	4.428225	2.038282	1.088060	1.769177
27	H	7.238851	5.985833	3.629372	1.088166	1.769276

		26	27
26	H	0.000000	
27	H	1.744468	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.657806	-1.007112	0.018246
2	6	0	-2.458059	-1.662258	-0.009270
3	6	0	-1.218111	-0.941506	-0.019055
4	6	0	-1.230691	0.505428	-0.012262
5	6	0	-2.524124	1.142963	0.024940
6	6	0	-3.687551	0.418100	0.038927
7	6	0	0.000305	-1.623775	-0.029356
8	6	0	-0.000137	1.220754	-0.029069
9	6	0	1.230854	0.505909	-0.012483
10	6	0	1.218507	-0.941116	-0.018110
11	6	0	2.458505	-1.661757	-0.006858
12	1	0	2.420442	-2.749107	-0.014774
13	6	0	3.658222	-1.006557	0.019189
14	6	0	3.687867	0.418652	0.037391
15	6	0	2.524380	1.143442	0.023183
16	1	0	0.000426	-2.712228	-0.031437
17	1	0	-4.593471	-1.560926	0.029146
18	1	0	-2.419955	-2.749589	-0.019255
19	1	0	-2.583042	2.222273	0.051179
20	1	0	-4.649483	0.924289	0.067115
21	1	0	4.593949	-1.560262	0.030501
22	1	0	4.649731	0.925010	0.064746

This journal is © The Royal Society of Chemistry 2014

```
     23          1           0        2.583529    2.222712    0.048217
     24          6           0       -0.001504    2.753886   -0.040744
     25          1           0       -0.004860    3.149562    0.981700
     26          1           0        0.871624    3.150065   -0.555103
     27          1           0       -0.872835    3.147869   -0.560037
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3847071      0.4464116
0.3383604
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       877.4318460248 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860059825     A.U. after   13 cycles
             Convg  =    0.2705D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.002798626   -0.000321085    0.000076772
      2        6           0.002041251    0.001414493    0.000026820
      3        6          -0.001212083   -0.001908638   -0.000035777
      4        6          -0.000717766    0.001845865    0.000288139
      5        6           0.005467820    0.002174141   -0.000470048
      6        6           0.000381152   -0.002218806   -0.000012962
      7        6           0.000142806   -0.000263877    0.000379600
      8        6          -0.002361402    0.004101844   -0.000661365
      9        6          -0.001324314    0.001531268    0.000255831
     10        6           0.002248648    0.000122647   -0.000037681
     11        6          -0.002224717   -0.001107367   -0.000016442
     12        1          -0.000142695    0.000050251   -0.000058915
     13        6           0.001660662    0.002296755    0.000069710
     14        6           0.001716430   -0.001400916    0.000045937
     15        6          -0.004578934   -0.003743645   -0.000457987
     16        1           0.000022483   -0.000021683   -0.000247756
     17        1           0.000610898   -0.000100208   -0.000084427
     18        1           0.000024196    0.000147202   -0.000033068
     19        1          -0.001247842    0.001954949    0.000091587
     20        1           0.000122279    0.001225044    0.000116138
     21        1          -0.000210989   -0.000589181   -0.000064257
     22        1          -0.001126034    0.000488775    0.000086587
     23        1          -0.001156574    0.002073240    0.000078422
```

```
     24        6           0.006745657   -0.011416884    0.001200755
     25        1          -0.000926108    0.001560217    0.000790635
     26        1           0.001601268    0.002332315   -0.000658396
     27        1          -0.002757465   -0.000226717   -0.000667853
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.011416884 RMS     0.002115448


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.009052962 RMS     0.001478171
 Search for a local minimum.
 Step number   2 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    1    2
 DE= -5.52D-03 DEPred=-6.46D-03 R= 8.54D-01
 SS=  1.41D+00  RLast= 2.28D-01 DXNew= 5.0454D-01 6.8337D-01
 Trust test= 8.54D-01 RLast= 2.28D-01 DXMaxT set to 5.05D-01
 Use linear search instead of GDIIS.
     Eigenvalues ---    0.00237   0.01348   0.01760   0.01762
0.01774
     Eigenvalues ---    0.01819   0.01823   0.01929   0.01977
0.01978
     Eigenvalues ---    0.02004   0.02010   0.02100   0.02109
0.02109
     Eigenvalues ---    0.02125   0.02149   0.02150   0.02222
0.02225
     Eigenvalues ---    0.02347   0.02350   0.06885   0.06892
0.15201
     Eigenvalues ---    0.15998   0.15999   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16216   0.21933   0.22000   0.22550
0.22569
     Eigenvalues ---    0.23552   0.24460   0.24609   0.24995
0.24998
     Eigenvalues ---    0.25497   0.27682   0.33199   0.33587
0.33630
     Eigenvalues ---    0.33631   0.33648   0.33681   0.33682
0.33683
     Eigenvalues ---    0.34190   0.35839   0.35883   0.37230
0.37257
     Eigenvalues ---    0.38329   0.38602   0.39411   0.40238
0.40624
     Eigenvalues ---    0.41160   0.41388   0.44418   0.44927
0.45765
     Eigenvalues ---    0.49802   0.49862   0.50734   0.51347
0.51711
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-7.76988495D-04 EMin= 2.36824309D-03
 Quartic linear search produced a step of -0.07602.
 Iteration  1 RMS(Cart)=  0.01308746 RMS(Int)=  0.00004105
 Iteration  2 RMS(Cart)=  0.00006121 RMS(Int)=  0.00000824
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000824
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58372   0.00211  -0.00038   0.00474   0.00436
2.58809
    R2        2.69413   0.00029   0.00002   0.00092   0.00094
2.69507
    R3        2.05477  -0.00021   0.00182  -0.00385  -0.00203
2.05274
    R4        2.71033  -0.00131  -0.00020  -0.00252  -0.00272
2.70760
    R5        2.05610  -0.00011   0.00178  -0.00351  -0.00173
2.05437
    R6        2.73444  -0.00013  -0.00262   0.00414   0.00152
2.73597
    R7        2.63895   0.00131   0.00038   0.00265   0.00304
2.64199
```

This journal is © The Royal Society of Chemistry 2014

R8	2.72593	-0.00484	-0.00139	-0.00889	-0.01028
2.71565					
R9	2.68995	-0.00610	-0.00350	-0.00666	-0.01016
2.67979					
R10	2.59050	0.00103	-0.00089	0.00337	0.00248
2.59298					
R11	2.04324	0.00232	0.00276	0.00139	0.00415
2.04739					
R12	2.05480	-0.00018	0.00182	-0.00375	-0.00194
2.05286					
R13	2.63897	0.00130	0.00038	0.00261	0.00300
2.64197					
R14	2.05688	0.00003	0.00180	-0.00315	-0.00136
2.05553					
R15	2.69020	-0.00628	-0.00351	-0.00700	-0.01052
2.67968					
R16	2.89729	-0.00905	0.00098	-0.03100	-0.03002
2.86726					
R17	2.73460	-0.00017	-0.00264	0.00404	0.00141
2.73601					
R18	2.72601	-0.00490	-0.00140	-0.00901	-0.01042
2.71559					
R19	2.71032	-0.00131	-0.00021	-0.00250	-0.00271
2.70761					
R20	2.05611	-0.00011	0.00179	-0.00352	-0.00174
2.05437					
R21	2.58367	0.00214	-0.00037	0.00478	0.00442
2.58809					
R22	2.69406	0.00033	0.00002	0.00101	0.00103
2.69508					
R23	2.05477	-0.00021	0.00182	-0.00385	-0.00203
2.05274					
R24	2.59053	0.00101	-0.00089	0.00334	0.00244
2.59297					
R25	2.05479	-0.00018	0.00182	-0.00376	-0.00194
2.05286					
R26	2.04313	0.00237	0.00277	0.00151	0.00429
2.04742					
R27	2.07178	0.00140	-0.00378	0.01028	0.00650
2.07828					
R28	2.05614	0.00280	-0.00259	0.01162	0.00902
2.06516					
R29	2.05634	0.00275	-0.00261	0.01150	0.00889
2.06523					
A1	2.09165	-0.00072	0.00080	-0.00304	-0.00223
2.08942					
A2	2.10742	-0.00024	0.00028	-0.00315	-0.00287
2.10455					
A3	2.08411	0.00096	-0.00108	0.00619	0.00510
2.08921					
A4	2.11526	-0.00031	-0.00057	0.00071	0.00015
2.11540					

A5	2.10572	0.00026	0.00067	-0.00045	0.00022
2.10593					
A6	2.06220	0.00005	-0.00010	-0.00026	-0.00036
2.06184					
A7	2.08858	-0.00063	-0.00116	-0.00113	-0.00230
2.08629					
A8	2.10462	0.00187	0.00148	0.00385	0.00533
2.10995					
A9	2.08997	-0.00124	-0.00031	-0.00272	-0.00302
2.08695					
A10	2.03741	0.00216	0.00272	0.00267	0.00539
2.04280					
A11	2.08855	0.00121	-0.00020	0.00389	0.00369
2.09224					
A12	2.15718	-0.00337	-0.00252	-0.00655	-0.00907
2.14811					
A13	2.12652	-0.00070	-0.00143	-0.00119	-0.00262
2.12390					
A14	2.08365	0.00031	-0.00174	0.00471	0.00297
2.08662					
A15	2.07298	0.00039	0.00317	-0.00355	-0.00039
2.07259					
A16	2.10685	0.00020	-0.00035	0.00196	0.00160
2.10846					
A17	2.07625	0.00115	-0.00053	0.00747	0.00694
2.08319					
A18	2.10008	-0.00135	0.00088	-0.00942	-0.00854
2.09154					
A19	2.12025	-0.00114	-0.00067	-0.00092	-0.00157
2.11867					
A20	2.08137	0.00058	0.00032	0.00056	0.00087
2.08224					
A21	2.08146	0.00056	0.00035	0.00041	0.00076
2.08222					
A22	2.08868	0.00115	0.00173	-0.00171	0.00001
2.08870					
A23	2.09651	-0.00042	-0.00083	0.00135	0.00053
2.09705					
A24	2.09785	-0.00073	-0.00089	0.00031	-0.00058
2.09727					
A25	2.08828	0.00128	-0.00019	0.00411	0.00392
2.09220					
A26	2.15765	-0.00351	-0.00256	-0.00694	-0.00950
2.14815					
A27	2.03720	0.00223	0.00275	0.00285	0.00560
2.04280					
A28	2.09012	-0.00126	-0.00032	-0.00281	-0.00312
2.08700					
A29	2.10440	0.00192	0.00150	0.00402	0.00551
2.10990					
A30	2.08866	-0.00066	-0.00118	-0.00120	-0.00238
2.08628					

```
   A31        2.06216   0.00006  -0.00010  -0.00024  -0.00035
2.06182
   A32        2.11532  -0.00033  -0.00057   0.00066   0.00009
2.11541
   A33        2.10569   0.00027   0.00068  -0.00042   0.00025
2.10594
   A34        2.09159  -0.00072   0.00081  -0.00301  -0.00219
2.08940
   A35        2.10750  -0.00025   0.00030  -0.00323  -0.00294
2.10456
   A36        2.08409   0.00096  -0.00110   0.00624   0.00513
2.08922
   A37        2.10689   0.00019  -0.00036   0.00195   0.00159
2.10847
   A38        2.07631   0.00115  -0.00051   0.00742   0.00692
2.08323
   A39        2.09999  -0.00134   0.00087  -0.00937  -0.00850
2.09149
   A40        2.12663  -0.00072  -0.00144  -0.00128  -0.00272
2.12391
   A41        2.08380   0.00028  -0.00175   0.00458   0.00283
2.08663
   A42        2.07272   0.00044   0.00319  -0.00334  -0.00014
2.07257
   A43        1.93242   0.00175  -0.00166   0.01215   0.01052
1.94294
   A44        1.94657  -0.00003  -0.00273   0.00498   0.00228
1.94884
   A45        1.94593   0.00003  -0.00268   0.00531   0.00265
1.94858
   A46        1.88800  -0.00106   0.00172  -0.01008  -0.00833
1.87967
   A47        1.88802  -0.00107   0.00172  -0.01000  -0.00826
1.87976
   A48        1.85994   0.00027   0.00385  -0.00385   0.00003
1.85997
    D1       -0.00097   0.00002   0.00029  -0.00018   0.00011  -
0.00085
    D2        3.13515   0.00003   0.00045   0.00014   0.00060
3.13575
    D3       -3.13769  -0.00001  -0.00010  -0.00044  -0.00054  -
3.13822
    D4       -0.00157   0.00000   0.00006  -0.00012  -0.00005  -
0.00161
    D5        0.00561   0.00004  -0.00042   0.00245   0.00203
0.00763
    D6       -3.13487   0.00005  -0.00063   0.00323   0.00260  -
3.13227
    D7       -3.14079   0.00006  -0.00004   0.00268   0.00265  -
3.13814
    D8        0.00191   0.00007  -0.00025   0.00346   0.00322
0.00513
```

D9	-0.01011	-0.00001	0.00043	-0.00159	-0.00115	-0.01126
D10	3.12673	0.00001	0.00082	-0.00093	-0.00010	3.12663
D11	3.13682	-0.00002	0.00027	-0.00190	-0.00163	3.13520
D12	-0.00952	0.00000	0.00065	-0.00124	-0.00058	-0.01010
D13	0.01599	0.00000	-0.00097	0.00120	0.00023	0.01622
D14	-3.13586	0.00003	-0.00033	0.00244	0.00209	-3.13376
D15	-3.12089	-0.00003	-0.00135	0.00053	-0.00082	-3.12171
D16	0.01045	0.00000	-0.00071	0.00176	0.00104	0.01149
D17	-3.12407	-0.00003	-0.00127	0.00050	-0.00079	-3.12486
D18	0.00162	0.00010	-0.00015	0.00451	0.00436	0.00598
D19	0.01277	-0.00001	-0.00089	0.00116	0.00026	0.01303
D20	3.13846	0.00013	0.00023	0.00518	0.00541	-3.13932
D21	-0.01174	0.00005	0.00086	0.00103	0.00188	-0.00987
D22	3.12052	-0.00002	0.00163	-0.00364	-0.00201	3.11851
D23	3.14055	0.00000	0.00019	-0.00033	-0.00013	3.14041
D24	-0.01037	-0.00008	0.00096	-0.00499	-0.00402	-0.01439
D25	-0.03227	-0.00005	0.00232	-0.00530	-0.00299	-0.03526
D26	3.12751	-0.00002	0.00107	-0.00222	-0.00114	3.12637
D27	3.09833	0.00002	0.00301	-0.00392	-0.00092	3.09741
D28	-0.02508	0.00005	0.00176	-0.00083	0.00093	-0.02415
D29	0.00109	-0.00008	-0.00017	-0.00289	-0.00307	-0.00198
D30	3.14155	-0.00009	0.00004	-0.00367	-0.00363	3.13792
D31	-3.13123	-0.00001	-0.00094	0.00171	0.00077	-3.13046
D32	0.00923	-0.00001	-0.00073	0.00093	0.00021	0.00944
D33	-0.01371	0.00002	0.00084	-0.00047	0.00038	-0.01333
D34	3.12366	0.00004	0.00123	-0.00011	0.00114	3.12479

This journal is © The Royal Society of Chemistry 2014

D35	-3.13940	-0.00011	-0.00028	-0.00449	-0.00477	3.13902
D36	-0.00203	-0.00010	0.00011	-0.00412	-0.00401	-0.00604
D37	0.03134	0.00006	-0.00237	0.00598	0.00362	0.03496
D38	-3.09942	-0.00001	-0.00310	0.00457	0.00149	-3.09792
D39	-3.12845	0.00003	-0.00111	0.00290	0.00179	-3.12666
D40	0.02398	-0.00003	-0.00184	0.00150	-0.00034	0.02363
D41	1.55864	0.00000	0.00063	-0.00379	-0.00316	1.55548
D42	-2.62121	-0.00018	-0.00005	-0.00495	-0.00500	-2.62621
D43	-0.54430	0.00015	0.00128	-0.00294	-0.00165	-0.54596
D44	-1.56468	0.00001	-0.00063	-0.00067	-0.00131	-1.56598
D45	0.53866	-0.00017	-0.00131	-0.00184	-0.00315	0.53551
D46	2.61557	0.00016	0.00002	0.00018	0.00019	2.61577
D47	-0.00857	-0.00002	0.00080	-0.00314	-0.00232	-0.01089
D48	3.13722	-0.00005	0.00042	-0.00351	-0.00309	3.13413
D49	3.12292	0.00000	0.00148	-0.00189	-0.00041	3.12251
D50	-0.01448	-0.00002	0.00110	-0.00227	-0.00118	-0.01566
D51	-3.14089	0.00001	-0.00017	0.00050	0.00032	-3.14057
D52	0.01020	0.00008	-0.00091	0.00484	0.00392	0.01412
D53	0.01125	-0.00005	-0.00088	-0.00088	-0.00175	0.00950
D54	-3.12084	0.00002	-0.00162	0.00347	0.00185	-3.11899
D55	0.00773	0.00003	-0.00073	0.00239	0.00166	0.00939
D56	-3.12879	0.00002	-0.00096	0.00251	0.00154	-3.12725
D57	-3.13809	0.00004	-0.00034	0.00276	0.00241	-3.13568
D58	0.00858	0.00004	-0.00057	0.00287	0.00229	0.01087
D59	0.00142	-0.00002	-0.00024	-0.00034	-0.00059	0.00083
D60	3.13846	-0.00001	0.00018	-0.00030	-0.00012	3.13833

```
   D61       -3.13497  -0.00003  -0.00048  -0.00023  -0.00072  -
3.13568
   D62        0.00206  -0.00001  -0.00005  -0.00019  -0.00024
0.00182
   D63       -0.00500  -0.00005   0.00048  -0.00288  -0.00239  -
0.00739
   D64        3.13454  -0.00003   0.00054  -0.00247  -0.00193
3.13261
   D65        3.14109  -0.00006   0.00007  -0.00289  -0.00284
3.13826
   D66       -0.00255  -0.00005   0.00012  -0.00249  -0.00237  -
0.00492
   D67       -0.00166   0.00009   0.00010   0.00349   0.00360
0.00194
   D68        3.13050   0.00002   0.00084  -0.00079   0.00004
3.13054
   D69       -3.14118   0.00008   0.00005   0.00306   0.00312  -
3.13806
   D70       -0.00902   0.00001   0.00079  -0.00122  -0.00044  -
0.00946
         Item               Value     Threshold  Converged?
 Maximum Force            0.009053     0.000450     NO
 RMS     Force            0.001478     0.000300     NO
 Maximum Displacement     0.056191     0.001800     NO
 RMS     Displacement     0.013089     0.001200     NO
 Predicted change in Energy=-4.290015D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.790901   -5.434299    0.002517
      2          6           0       -3.421980   -5.399427   -0.020378
      3          6           0       -2.711189   -4.155406   -0.030792
      4          6           0       -3.450831   -2.910783   -0.031085
      5          6           0       -4.884605   -3.002771    0.000091
      6          6           0       -5.528993   -4.214070    0.017410
      7          6           0       -1.313401   -4.127389   -0.036227
      8          6           0       -2.754790   -1.675435   -0.050989
      9          6           0       -1.336985   -1.668049   -0.027057
     10          6           0       -0.609197   -2.919666   -0.026416
     11          6           0        0.823443   -2.903645   -0.011463
     12          1           0        1.346824   -3.856476   -0.016966
     13          6           0        1.519619   -1.724526    0.015004
     14          6           0        0.812332   -0.486170    0.029080
     15          6           0       -0.559395   -0.460076    0.007720
     16          1           0       -0.762124   -5.065079   -0.038143
     17          1           0       -5.319457   -6.383234    0.013383
```

This journal is © The Royal Society of Chemistry 2014

18	1	0	-2.843981	-6.320148	-0.026509
19	1	0	-5.477886	-2.096502	0.022778
20	1	0	-6.614441	-4.248489	0.044375
21	1	0	2.605788	-1.724218	0.029197
22	1	0	1.370183	0.445514	0.058569
23	1	0	-1.062772	0.499081	0.029836
24	6	0	-3.523795	-0.367619	-0.071387
25	1	0	-3.739544	-0.014641	0.947618
26	1	0	-2.966634	0.419966	-0.584776
27	1	0	-4.476720	-0.468456	-0.596873

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.369556	0.000000			
3	C	2.441696	1.432802	0.000000		
4	C	2.857455	2.488834	1.447811	0.000000	
5	C	2.433334	2.807784	2.460336	1.437059	0.000000
6	C	1.426170	2.417851	2.818826	2.453500	1.372144
7	C	3.715174	2.462608	1.398079	2.459423	3.744273
8	C	4.275240	3.783411	2.480436	1.418082	2.510088
9	C	5.110289	4.274393	2.841724	2.452091	3.790492
10	C	4.879638	3.749800	2.438328	2.841652	4.276298
11	C	6.158349	4.924696	3.749788	4.274326	5.708920
12	H	6.337317	5.012206	4.069033	4.889993	6.289659
13	C	7.320193	6.158372	4.879653	5.110255	6.530560
14	C	7.475354	6.486289	5.087443	4.904787	6.228099
15	C	6.530587	5.708973	4.276350	3.790498	5.017250
16	H	4.045865	2.680847	2.150911	3.445314	4.609710
17	H	1.086263	2.137623	3.430485	3.943559	3.408343
18	H	2.139175	1.087128	2.168815	3.462955	3.894848
19	H	3.407822	3.890749	3.449139	2.185156	1.083430
20	H	2.175591	3.394209	3.905084	3.435633	2.132159
21	H	8.275048	7.060001	5.846753	6.172051	7.598785
22	H	8.516707	7.558730	6.150939	5.874943	7.142581
23	H	7.007474	6.353014	4.938137	4.163377	5.183653
24	C	5.223243	5.033097	3.874184	2.544530	2.966638
25	H	5.601005	5.480309	4.377297	3.070644	3.337348
26	H	6.159975	5.864404	4.615862	3.410999	3.966840
27	H	5.011744	5.075362	4.126881	2.708787	2.635430

		6	7	8	9	10
6	C	0.000000				
7	C	4.216824	0.000000			
8	C	3.761057	2.844274	0.000000		
9	C	4.904807	2.459470	1.418026	0.000000	
10	C	5.087416	1.398068	2.480380	1.447833	0.000000
11	C	6.486254	2.462573	3.783360	2.488853	1.432808
12	H	6.885196	2.674054	4.645572	3.462967	2.168806
13	C	7.475344	3.715155	4.275200	2.857471	2.441706
14	C	7.355935	4.216809	3.761000	2.453478	2.818816
15	C	6.228119	3.744281	2.510040	1.437030	2.460331
16	H	4.842556	1.087738	3.931993	3.445344	2.150889

This journal is © The Royal Society of Chemistry 2014

17	H	2.179265	4.597802	5.361440	6.172090	5.846746
18	H	3.412739	2.674128	4.645634	4.890098	4.069095
19	H	2.118191	4.633672	2.756445	4.163306	4.938031
20	H	1.086328	5.303035	4.639677	5.874973	6.150913
21	H	8.507301	4.597777	5.361399	3.943574	3.430498
22	H	8.325386	5.303023	4.639593	3.435584	3.905074
23	H	6.493156	4.633724	2.756442	2.185151	3.449163
24	C	4.338651	4.361530	1.517289	2.544646	3.874254
25	H	4.658607	4.875327	2.173750	3.075067	4.380295
26	H	5.329409	4.869550	2.172674	2.706772	4.125823
27	H	3.938813	4.869158	2.172517	3.409054	4.614280

		11	12	13	14	15
11	C	0.000000				
12	H	1.087126	0.000000			
13	C	1.369556	2.139180	0.000000		
14	C	2.417841	3.412735	1.426176	0.000000	
15	C	2.807783	3.894845	2.433349	1.372142	0.000000
16	H	2.680770	2.430809	4.045796	4.842503	4.609692
17	H	7.059984	7.129147	8.275054	8.507317	7.598818
18	H	5.012256	4.861339	6.337386	6.885275	6.289749
19	H	6.352905	7.048103	7.007389	6.493077	5.183596
20	H	7.558693	7.971147	8.516699	8.325397	7.142618
21	H	2.137628	2.476620	1.086262	2.179276	3.408357
22	H	3.394216	4.302717	2.175616	1.086325	2.132123
23	H	3.890766	4.977873	3.407843	2.118192	1.083448
24	C	5.033239	5.991495	5.223473	4.338910	2.966896
25	H	5.485165	6.446802	5.608232	4.667508	3.345918
26	H	5.073437	6.100515	5.008497	3.934271	2.630651
27	H	5.862131	6.762295	6.156962	5.325993	3.963715

		16	17	18	19	20
16	H	0.000000				
17	H	4.744415	0.000000			
18	H	2.430938	2.476602	0.000000		
19	H	5.572663	4.289669	4.977858	0.000000	
20	H	5.909589	2.497015	4.302693	2.433777	0.000000
21	H	4.744335	9.193269	7.129211	8.092244	9.559539
22	H	5.909545	9.559557	7.971235	7.304736	9.262185
23	H	5.572691	8.092336	7.048245	5.121555	7.304837
24	C	5.449226	6.278472	5.991390	2.610819	4.962524
25	H	5.945055	6.627812	6.442854	2.865538	5.196763
26	H	5.936699	7.223372	6.764307	3.606677	5.957919
27	H	5.936274	6.005599	6.101922	2.009188	4.389726

		21	22	23	24	25
21	H	0.000000				
22	H	2.497062	0.000000			
23	H	4.289684	2.433715	0.000000		
24	C	6.278715	4.962770	2.611139	0.000000	
25	H	6.635464	5.206866	2.875993	1.099779	0.000000
26	H	6.002197	4.384350	2.002172	1.092834	1.770453
27	H	7.220167	5.954092	3.603322	1.092872	1.770545

		26	27
26	H	0.000000	

```
   27  H    1.752084   0.000000
 Stoichiometry    C15H12
 Framework group  C1[X(C15H12)]
 Deg. of freedom    75
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.660079   -0.996234    0.018842
      2          6           0       -2.462336   -1.659795   -0.009119
      3          6           0       -1.219152   -0.947524   -0.018272
      4          6           0       -1.226024    0.500256   -0.011818
      5          6           0       -2.508607    1.147406    0.024489
      6          6           0       -3.677953    0.429661    0.040399
      7          6           0        0.000032   -1.631704   -0.028905
      8          6           0        0.000034    1.212570   -0.030432
      9          6           0        1.226067    0.500323   -0.011839
     10          6           0        1.219177   -0.947481   -0.017924
     11          6           0        2.462360   -1.659760   -0.008338
     12          1           0        2.430666   -2.746373   -0.018844
     13          6           0        3.660114   -0.996203    0.019239
     14          6           0        3.677982    0.429710    0.039920
     15          6           0        2.508643    1.147457    0.023831
     16          1           0        0.000066   -2.719420   -0.035881
     17          1           0       -4.596619   -1.546475    0.028695
     18          1           0       -2.430673   -2.746404   -0.020358
     19          1           0       -2.560740    2.229224    0.052295
     20          1           0       -4.631085    0.949938    0.071360
     21          1           0        4.596650   -1.546443    0.029325
     22          1           0        4.631100    0.950046    0.070257
     23          1           0        2.560815    2.229309    0.050895
     24          6           0       -0.000160    2.729800   -0.043771
     25          1           0       -0.005585    3.138685    0.977158
     26          1           0        0.878440    3.128788   -0.556761
     27          1           0       -0.873620    3.128232   -0.565966
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3917031      0.4477535
0.3395530
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.6584178241 Hartrees.
```

```
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
```

This journal is © The Royal Society of Chemistry 2014

```
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860532026     A.U. after   11 cycles
            Convg  =    0.9411D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000735744    0.001203581    0.000036266
      2        6           0.000330543    0.001322234    0.000016541
      3        6          -0.000319324   -0.000576963   -0.000048204
      4        6          -0.000296345   -0.000275948    0.000003204
      5        6           0.001603044    0.000205313    0.000015046
      6        6           0.000643104   -0.001391179   -0.000037034
      7        6          -0.000431796    0.000747299    0.000093659
      8        6          -0.000503353    0.000834413   -0.000037736
      9        6           0.000378764    0.000118523   -0.000019349
     10        6           0.000670274   -0.000018273   -0.000056656
     11        6          -0.001308438    0.000362009    0.000021096
     12        1           0.000315173   -0.000433456   -0.000016396
     13        6          -0.000698300    0.001218635    0.000034591
     14        6           0.000888952   -0.001230815   -0.000042537
     15        6          -0.000896032   -0.001275287    0.000025064
     16        1           0.000261283   -0.000445461   -0.000049434
     17        1          -0.000079666   -0.000461444   -0.000025662
     18        1           0.000226414   -0.000484691   -0.000004761
     19        1          -0.000404745    0.000285018    0.000067264
     20        1          -0.000573289    0.000204210    0.000038264
     21        1           0.000442092   -0.000154829   -0.000021130
     22        1           0.000105344    0.000599002    0.000042876
     23        1           0.000006022    0.000466543    0.000081118
     24        6           0.001089108   -0.001852902   -0.000254315
     25        1          -0.000274610    0.000452441   -0.000630873
     26        1          -0.000633747    0.000048687    0.000387924
     27        1           0.000195274    0.000533341    0.000381175
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.001852902 RMS     0.000600071


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000985315 RMS     0.000290444
 Search for a local minimum.
 Step number   3 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
```

This journal is © The Royal Society of Chemistry 2014

```
 Update second derivatives using D2CorX and points    1    2    3
 DE= -4.72D-04 DEPred=-4.29D-04 R= 1.10D+00
 SS=  1.41D+00  RLast= 5.49D-02 DXNew= 8.4853D-01 1.6461D-01
 Trust test= 1.10D+00 RLast= 5.49D-02 DXMaxT set to 5.05D-01
 Use linear search instead of GDIIS.
     Eigenvalues ---    0.00237   0.01350   0.01759   0.01760
0.01773
     Eigenvalues ---    0.01819   0.01822   0.01925   0.01976
0.01978
     Eigenvalues ---    0.02004   0.02009   0.02095   0.02109
0.02110
     Eigenvalues ---    0.02119   0.02147   0.02147   0.02222
0.02225
     Eigenvalues ---    0.02345   0.02349   0.06809   0.06844
0.13408
     Eigenvalues ---    0.15999   0.15999   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16028
     Eigenvalues ---    0.16257   0.21983   0.22000   0.22470
0.22571
     Eigenvalues ---    0.23515   0.24458   0.24610   0.24988
0.24998
     Eigenvalues ---    0.25475   0.28107   0.33585   0.33630
0.33631
     Eigenvalues ---    0.33647   0.33676   0.33682   0.33682
0.33938
     Eigenvalues ---    0.34209   0.35827   0.36712   0.37231
0.37291
     Eigenvalues ---    0.38342   0.38607   0.39371   0.40121
0.40235
     Eigenvalues ---    0.41160   0.41950   0.44448   0.44930
0.45766
     Eigenvalues ---    0.49525   0.49862   0.50231   0.51049
0.51348
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-4.97459193D-05 EMin= 2.36888516D-03
 Quartic linear search produced a step of  0.10501.
 Iteration  1 RMS(Cart)=  0.00519377 RMS(Int)=  0.00001223
 Iteration  2 RMS(Cart)=  0.00001481 RMS(Int)=  0.00000230
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000230
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58809   0.00038   0.00046   0.00065   0.00111
2.58920
    R2        2.69507  -0.00097   0.00010  -0.00257  -0.00247
2.69260
    R3        2.05274   0.00044  -0.00021   0.00136   0.00115
2.05389
    R4        2.70760  -0.00070  -0.00029  -0.00179  -0.00208
2.70553
    R5        2.05437   0.00053  -0.00018   0.00165   0.00146
2.05584
    R6        2.73597  -0.00037   0.00016  -0.00087  -0.00071
2.73526
    R7        2.64199  -0.00009   0.00032  -0.00040  -0.00008
2.64191
    R8        2.71565  -0.00084  -0.00108  -0.00162  -0.00270
2.71295
    R9        2.67979  -0.00032  -0.00107   0.00014  -0.00093
2.67886
   R10        2.59298   0.00045   0.00026   0.00096   0.00122
2.59420
   R11        2.04739   0.00046   0.00044   0.00099   0.00143
2.04881
   R12        2.05286   0.00057  -0.00020   0.00177   0.00157
2.05443
   R13        2.64197  -0.00008   0.00031  -0.00037  -0.00005
2.64191
   R14        2.05553   0.00052  -0.00014   0.00158   0.00144
2.05696
   R15        2.67968  -0.00018  -0.00110   0.00051  -0.00060
2.67908
```

This journal is © The Royal Society of Chemistry 2014

R16	2.86726	-0.00089	-0.00315	-0.00196	-0.00512
2.86215					
R17	2.73601	-0.00031	0.00015	-0.00065	-0.00050
2.73551					
R18	2.71559	-0.00076	-0.00109	-0.00137	-0.00247
2.71313					
R19	2.70761	-0.00070	-0.00028	-0.00178	-0.00206
2.70555					
R20	2.05437	0.00053	-0.00018	0.00165	0.00147
2.05584					
R21	2.58809	0.00036	0.00046	0.00058	0.00105
2.58913					
R22	2.69508	-0.00099	0.00011	-0.00263	-0.00252
2.69256					
R23	2.05274	0.00044	-0.00021	0.00136	0.00115
2.05389					
R24	2.59297	0.00044	0.00026	0.00094	0.00120
2.59417					
R25	2.05286	0.00057	-0.00020	0.00177	0.00157
2.05443					
R26	2.04742	0.00041	0.00045	0.00082	0.00127
2.04869					
R27	2.07828	-0.00039	0.00068	-0.00107	-0.00039
2.07789					
R28	2.06516	-0.00047	0.00095	-0.00159	-0.00065
2.06451					
R29	2.06523	-0.00040	0.00093	-0.00138	-0.00045
2.06478					
A1	2.08942	-0.00009	-0.00023	-0.00029	-0.00053
2.08889					
A2	2.10455	-0.00011	-0.00030	-0.00081	-0.00111
2.10344					
A3	2.08921	0.00021	0.00054	0.00110	0.00164
2.09085					
A4	2.11540	0.00017	0.00002	0.00088	0.00089
2.11630					
A5	2.10593	-0.00015	0.00002	-0.00097	-0.00094
2.10499					
A6	2.06184	-0.00002	-0.00004	0.00009	0.00005
2.06189					
A7	2.08629	-0.00011	-0.00024	-0.00040	-0.00064
2.08565					
A8	2.10995	0.00024	0.00056	0.00074	0.00130
2.11125					
A9	2.08695	-0.00013	-0.00032	-0.00034	-0.00066
2.08628					
A10	2.04280	0.00008	0.00057	-0.00037	0.00020
2.04300					
A11	2.09224	0.00019	0.00039	0.00060	0.00099
2.09323					
A12	2.14811	-0.00027	-0.00095	-0.00024	-0.00119
2.14692					

This journal is © The Royal Society of Chemistry 2014

A13	2.12390	0.00014	-0.00028	0.00099	0.00071
2.12461					
A14	2.08662	0.00012	0.00031	0.00097	0.00128
2.08791					
A15	2.07259	-0.00026	-0.00004	-0.00197	-0.00201
2.07058					
A16	2.10846	-0.00019	0.00017	-0.00084	-0.00067
2.10779					
A17	2.08319	0.00032	0.00073	0.00164	0.00237
2.08556					
A18	2.09154	-0.00013	-0.00090	-0.00080	-0.00170
2.08984					
A19	2.11867	0.00005	-0.00017	0.00038	0.00022
2.11889					
A20	2.08224	-0.00002	0.00009	-0.00020	-0.00011
2.08213					
A21	2.08222	-0.00002	0.00008	-0.00019	-0.00011
2.08211					
A22	2.08870	-0.00012	0.00000	-0.00085	-0.00086
2.08784					
A23	2.09705	-0.00011	0.00006	-0.00033	-0.00027
2.09678					
A24	2.09727	0.00022	-0.00006	0.00121	0.00115
2.09842					
A25	2.09220	0.00011	0.00041	0.00028	0.00069
2.09289					
A26	2.14815	-0.00011	-0.00100	0.00040	-0.00059
2.14756					
A27	2.04280	0.00001	0.00059	-0.00069	-0.00011
2.04269					
A28	2.08700	-0.00011	-0.00033	-0.00020	-0.00053
2.08647					
A29	2.10990	0.00019	0.00058	0.00047	0.00105
2.11096					
A30	2.08628	-0.00008	-0.00025	-0.00027	-0.00052
2.08576					
A31	2.06182	-0.00002	-0.00004	0.00007	0.00003
2.06185					
A32	2.11541	0.00018	0.00001	0.00094	0.00095
2.11636					
A33	2.10594	-0.00016	0.00003	-0.00101	-0.00098
2.10496					
A34	2.08940	-0.00010	-0.00023	-0.00035	-0.00058
2.08882					
A35	2.10456	-0.00011	-0.00031	-0.00078	-0.00109
2.10347					
A36	2.08922	0.00021	0.00054	0.00113	0.00166
2.09089					
A37	2.10847	-0.00017	0.00017	-0.00080	-0.00063
2.10784					
A38	2.08323	0.00031	0.00073	0.00158	0.00231
2.08554					

This journal is © The Royal Society of Chemistry 2014

A39	2.09149	-0.00014	-0.00089	-0.00079	-0.00168	2.08981
A40	2.12391	0.00017	-0.00029	0.00114	0.00085	2.12476
A41	2.08663	0.00015	0.00030	0.00119	0.00149	2.08812
A42	2.07257	-0.00031	-0.00002	-0.00234	-0.00236	2.07022
A43	1.94294	0.00076	0.00110	0.00474	0.00583	1.94877
A44	1.94884	0.00054	0.00024	0.00400	0.00423	1.95307
A45	1.94858	0.00047	0.00028	0.00340	0.00367	1.95225
A46	1.87967	-0.00069	-0.00087	-0.00450	-0.00538	1.87429
A47	1.87976	-0.00070	-0.00087	-0.00478	-0.00566	1.87410
A48	1.85997	-0.00051	0.00000	-0.00376	-0.00377	1.85620
D1	-0.00085	-0.00001	0.00001	-0.00057	-0.00056	-0.00141
D2	3.13575	-0.00001	0.00006	-0.00063	-0.00057	3.13518
D3	-3.13822	-0.00001	-0.00006	-0.00031	-0.00036	-3.13859
D4	-0.00161	-0.00001	-0.00001	-0.00037	-0.00037	-0.00199
D5	0.00763	0.00002	0.00021	0.00077	0.00098	0.00862
D6	-3.13227	0.00002	0.00027	0.00127	0.00155	-3.13073
D7	-3.13814	0.00001	0.00028	0.00051	0.00078	-3.13736
D8	0.00513	0.00002	0.00034	0.00101	0.00135	0.00648
D9	-0.01126	-0.00001	-0.00012	-0.00073	-0.00085	-0.01211
D10	3.12663	-0.00002	-0.00001	-0.00108	-0.00109	3.12554
D11	3.13520	-0.00001	-0.00017	-0.00067	-0.00084	3.13436
D12	-0.01010	-0.00002	-0.00006	-0.00101	-0.00107	-0.01117
D13	0.01622	0.00003	0.00002	0.00176	0.00179	0.01801
D14	-3.13376	0.00002	0.00022	0.00089	0.00111	-3.13265
D15	-3.12171	0.00004	-0.00009	0.00210	0.00202	-3.11970
D16	0.01149	0.00003	0.00011	0.00123	0.00134	0.01283

This journal is © The Royal Society of Chemistry 2014

D17	-3.12486	0.00004	-0.00008	0.00173	0.00165	-3.12320
D18	0.00598	0.00003	0.00046	0.00093	0.00139	0.00737
D19	0.01303	0.00003	0.00003	0.00139	0.00142	0.01445
D20	-3.13932	0.00002	0.00057	0.00058	0.00115	-3.13816
D21	-0.00987	-0.00002	0.00020	-0.00161	-0.00141	-0.01127
D22	3.11851	-0.00004	-0.00021	-0.00228	-0.00249	3.11602
D23	3.14041	-0.00002	-0.00001	-0.00071	-0.00072	3.13969
D24	-0.01439	-0.00003	-0.00042	-0.00138	-0.00181	-0.01620
D25	-0.03526	-0.00008	-0.00031	-0.00396	-0.00427	-0.03953
D26	3.12637	-0.00011	-0.00012	-0.00598	-0.00610	3.12027
D27	3.09741	-0.00009	-0.00010	-0.00489	-0.00498	3.09243
D28	-0.02415	-0.00012	0.00010	-0.00691	-0.00681	-0.03096
D29	-0.00198	0.00000	-0.00032	0.00036	0.00003	-0.00195
D30	3.13792	-0.00001	-0.00038	-0.00015	-0.00053	3.13739
D31	-3.13046	0.00001	0.00008	0.00101	0.00109	-3.12938
D32	0.00944	0.00001	0.00002	0.00050	0.00052	0.00996
D33	-0.01333	-0.00003	0.00004	-0.00121	-0.00117	-0.01450
D34	3.12479	-0.00004	0.00012	-0.00183	-0.00171	3.12308
D35	3.13902	-0.00001	-0.00050	-0.00040	-0.00090	3.13812
D36	-0.00604	-0.00003	-0.00042	-0.00102	-0.00145	-0.00749
D37	0.03496	0.00009	0.00038	0.00414	0.00452	0.03948
D38	-3.09792	0.00010	0.00016	0.00560	0.00576	-3.09217
D39	-3.12666	0.00011	0.00019	0.00614	0.00633	-3.12034
D40	0.02363	0.00013	-0.00004	0.00760	0.00757	0.03120
D41	1.55548	0.00000	-0.00033	0.00401	0.00368	1.55916
D42	-2.62621	0.00001	-0.00053	0.00429	0.00376	-2.62245

This journal is © The Royal Society of Chemistry 2014

D43	-0.54596	0.00004	-0.00017	0.00451	0.00434	-0.54162
D44	-1.56598	-0.00002	-0.00014	0.00200	0.00186	-1.56412
D45	0.53551	-0.00002	-0.00033	0.00228	0.00195	0.53746
D46	2.61577	0.00002	0.00002	0.00250	0.00252	2.61829
D47	-0.01089	-0.00003	-0.00024	-0.00160	-0.00184	-0.01273
D48	3.13413	-0.00002	-0.00032	-0.00098	-0.00131	3.13282
D49	3.12251	-0.00005	-0.00004	-0.00297	-0.00301	3.11950
D50	-0.01566	-0.00004	-0.00012	-0.00235	-0.00248	-0.01813
D51	-3.14057	0.00001	0.00003	0.00069	0.00072	-3.13985
D52	0.01412	0.00004	0.00041	0.00161	0.00203	0.01615
D53	0.00950	0.00003	-0.00018	0.00211	0.00192	0.01143
D54	-3.11899	0.00005	0.00019	0.00303	0.00323	-3.11576
D55	0.00939	0.00003	0.00017	0.00166	0.00183	0.01122
D56	-3.12725	0.00003	0.00016	0.00166	0.00182	-3.12543
D57	-3.13568	0.00002	0.00025	0.00103	0.00129	-3.13439
D58	0.01087	0.00002	0.00024	0.00104	0.00128	0.01215
D59	0.00083	0.00001	-0.00006	0.00067	0.00061	0.00144
D60	3.13833	0.00000	-0.00001	0.00019	0.00018	3.13851
D61	-3.13568	0.00001	-0.00008	0.00067	0.00060	-3.13509
D62	0.00182	0.00001	-0.00003	0.00019	0.00017	0.00198
D63	-0.00739	-0.00002	-0.00025	-0.00098	-0.00123	-0.00862
D64	3.13261	-0.00003	-0.00020	-0.00171	-0.00191	3.13070
D65	3.13826	-0.00001	-0.00030	-0.00050	-0.00079	3.13746
D66	-0.00492	-0.00002	-0.00025	-0.00123	-0.00148	-0.00640
D67	0.00194	0.00000	0.00038	-0.00047	-0.00009	0.00185
D68	3.13054	-0.00002	0.00000	-0.00136	-0.00135	3.12918

```
   D69       -3.13806   0.00001   0.00033   0.00026   0.00059  -
3.13746
   D70       -0.00946  -0.00001  -0.00005  -0.00063  -0.00067  -
0.01013
         Item               Value     Threshold  Converged?
 Maximum Force            0.000985     0.000450     NO
 RMS     Force            0.000290     0.000300     YES
 Maximum Displacement     0.023041     0.001800     NO
 RMS     Displacement     0.005199     0.001200     NO
 Predicted change in Energy=-2.961459D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.791771   -5.432849    0.004188
      2          6           0       -3.422308   -5.398330   -0.021809
      3          6           0       -2.710623   -4.156090   -0.032663
      4          6           0       -3.449407   -2.911396   -0.031156
      5          6           0       -4.881719   -3.002228    0.004440
      6          6           0       -5.528145   -4.213160    0.022601
      7          6           0       -1.312888   -4.127892   -0.039972
      8          6           0       -2.754220   -1.676161   -0.052830
      9          6           0       -1.336759   -1.669206   -0.027171
     10          6           0       -0.608568   -2.920280   -0.028643
     11          6           0        0.822964   -2.902938   -0.013543
     12          1           0        1.347670   -3.855904   -0.021888
     13          6           0        1.519399   -1.723415    0.016540
     14          6           0        0.812030   -0.486703    0.035037
     15          6           0       -0.560349   -0.462191    0.012910
     16          1           0       -0.761216   -5.066224   -0.044335
     17          1           0       -5.319820   -6.382761    0.014996
     18          1           0       -2.845046   -6.320409   -0.030121
     19          1           0       -5.475780   -2.095671    0.030990
     20          1           0       -6.614420   -4.244182    0.053495
     21          1           0        2.606176   -1.724310    0.030618
     22          1           0        1.367568    0.447172    0.069200
     23          1           0       -1.062986    0.497989    0.039858
     24          6           0       -3.522847   -0.371373   -0.079281
     25          1           0       -3.741446   -0.008541    0.935425
     26          1           0       -2.970143    0.416804   -0.595842
     27          1           0       -4.476776   -0.471766   -0.602529
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                      1          2          3          4          5
    1  C    0.000000
    2  C    1.370144   0.000000
    3  C    2.441853   1.431703   0.000000
```

This journal is © The Royal Society of Chemistry 2014

4	C	2.856732	2.487099	1.447435	0.000000	
5	C	2.432285	2.805686	2.458950	1.435631	0.000000
6	C	1.424861	2.416847	2.818643	2.453290	1.372791
7	C	3.715843	2.462519	1.398039	2.458588	3.742412
8	C	4.274058	3.781778	2.480394	1.417589	2.507585
9	C	5.109119	4.272694	2.841149	2.450782	3.787438
10	C	4.879883	3.749388	2.438416	2.840854	4.274064
11	C	6.158409	4.924366	3.749265	4.272415	5.705575
12	H	6.338783	5.013159	4.069394	4.889185	6.287666
13	C	7.320581	6.158485	4.879898	5.109070	6.527619
14	C	7.474483	6.485131	5.087049	4.903403	6.224755
15	C	6.527821	5.705916	4.274417	3.787770	5.012594
16	H	4.047485	2.681830	2.151433	3.445262	4.608796
17	H	1.086870	2.137993	3.430488	3.943470	3.408820
18	H	2.139785	1.087902	2.168491	3.462170	3.893528
19	H	3.406662	3.889356	3.448982	2.185282	1.084186
20	H	2.176560	3.395189	3.905742	3.435228	2.132395
21	H	8.275480	7.060014	5.846872	6.171149	7.596205
22	H	8.515651	7.557849	6.150775	5.873099	7.138356
23	H	7.005708	6.351124	4.937653	4.162205	5.180298
24	C	5.218781	5.028291	3.871171	2.541540	2.962252
25	H	5.602990	5.483426	4.382003	3.073456	3.336033
26	H	6.156038	5.860866	4.614746	3.409616	3.962857
27	H	5.007961	5.071505	4.125323	2.708089	2.633558

		6	7	8	9	10
6	C	0.000000				
7	C	4.216585	0.000000			
8	C	3.759882	2.844044	0.000000		
9	C	4.903254	2.458835	1.417710	0.000000	
10	C	5.086885	1.398041	2.480371	1.447568	0.000000
11	C	6.484950	2.462330	3.781900	2.487305	1.431717
12	H	6.885234	2.674485	4.645184	3.462346	2.168480
13	C	7.474406	3.715716	4.274443	2.857006	2.441879
14	C	7.354214	4.216534	3.760408	2.453462	2.818591
15	C	6.224859	3.742522	2.508210	1.435724	2.458913
16	H	4.843120	1.088498	3.932514	3.445472	2.151423
17	H	2.179593	4.598148	5.360876	6.171237	5.846929
18	H	3.412082	2.674834	4.645191	4.889645	4.069730
19	H	2.118153	4.632994	2.754978	4.161340	4.936931
20	H	1.087157	5.303632	4.637584	5.872880	6.150587
21	H	8.506564	4.597961	5.361262	3.943744	3.430516
22	H	8.322963	5.303580	4.638164	3.435363	3.905691
23	H	6.490984	4.633314	2.756046	2.185446	3.449022
24	C	4.334851	4.358543	1.514582	2.542846	3.872017
25	H	4.658794	4.880404	2.175366	3.076835	4.384356
26	H	5.325637	4.869266	2.173014	2.709754	4.127334
27	H	3.936266	4.867640	2.172541	3.409488	4.613849

		11	12	13	14	15
11	C	0.000000				
12	H	1.087902	0.000000			
13	C	1.370110	2.139738	0.000000		
14	C	2.416748	3.411989	1.424840	0.000000	

15	C	2.805619	3.893460	2.432293	1.372776	0.000000
16	H	2.681488	2.431621	4.047132	4.842873	4.608768
17	H	7.060013	7.130343	8.275532	8.506674	7.596429
18	H	5.013350	4.863406	6.338998	6.885534	6.288116
19	H	6.350420	7.047034	7.005092	6.490405	5.179773
20	H	7.557652	7.971908	8.515553	8.322929	7.138409
21	H	2.137981	2.475942	1.086869	2.179599	3.408833
22	H	3.395096	4.304086	2.176528	1.087157	2.132362
23	H	3.889211	4.977093	3.406448	2.117859	1.084120
24	C	5.029832	5.988922	5.221249	4.337918	2.965323
25	H	5.487432	6.451182	5.609066	4.666206	3.343084
26	H	5.074192	6.101555	5.011141	3.939438	2.636346
27	H	5.860439	6.761191	6.156621	5.327118	3.964500

		16	17	18	19	20
16	H	0.000000				
17	H	4.745278	0.000000			
18	H	2.432185	2.475971	0.000000		
19	H	5.572878	4.289956	4.977239	0.000000	
20	H	5.911457	2.500199	4.304172	2.431688	0.000000
21	H	4.744822	9.193630	7.130472	8.090484	9.558749
22	H	5.911188	9.558874	7.972209	7.300611	9.258573
23	H	5.573026	8.091105	7.047778	5.118584	7.301150
24	C	5.446967	6.274934	5.987726	2.607549	4.957227
25	H	5.951626	6.630923	6.447905	2.860425	5.193499
26	H	5.936928	7.219986	6.762080	3.603285	5.952074
27	H	5.935150	6.002660	6.098919	2.009085	4.385317

		21	22	23	24	25
21	H	0.000000				
22	H	2.500195	0.000000			
23	H	4.289691	2.431262	0.000000		
24	C	6.277535	4.960667	2.611685	0.000000	
25	H	6.637382	5.201926	2.869279	1.099573	0.000000
26	H	6.006011	4.388501	2.011953	1.092492	1.766524
27	H	7.220662	5.954160	3.606528	1.092634	1.766520

		26	27
26	H	0.000000	
27	H	1.749155	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.660022	-0.994862	0.020722
2	6	0	-2.461877	-1.658778	-0.010260
3	6	0	-1.218953	-0.948272	-0.020046
4	6	0	-1.225307	0.499127	-0.012074

```
      5          6          0       -2.506151    1.146290    0.028572
      6          6          0       -3.676938    0.429682    0.045516
      7          6          0        0.000397   -1.632045   -0.032463
      8          6          0       -0.000174    1.212000   -0.032639
      9          6          0        1.225475    0.499772   -0.012226
     10          6          0        1.219463   -0.947761   -0.020143
     11          6          0        2.462489   -1.658115   -0.010309
     12          1          0        2.432059   -2.745512   -0.023452
     13          6          0        3.660560   -0.994137    0.020711
     14          6          0        3.677276    0.430388    0.045531
     15          6          0        2.506443    1.146890    0.028576
     16          1          0        0.000635   -2.720503   -0.041681
     17          1          0       -4.596520   -1.546368    0.030653
     18          1          0       -2.431347   -2.746172   -0.023472
     19          1          0       -2.558998    2.228729    0.060038
     20          1          0       -4.629148    0.953124    0.080352
     21          1          0        4.597110   -1.545552    0.030748
     22          1          0        4.629425    0.953941    0.080420
     23          1          0        2.559586    2.229243    0.060261
     24          6          0       -0.001859    2.726453   -0.052335
     25          1          0       -0.004793    3.145493    0.964256
     26          1          0        0.873101    3.128281   -0.568588
     27          1          0       -0.876048    3.125507   -0.572333
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3931605      0.4479352
0.3397609
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9012888160 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860563660     A.U. after   11 cycles
             Convg  =    0.3523D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000166720    0.000228700    0.000008191
      2        6           0.000137154    0.000122360   -0.000007974
      3        6           0.000018817   -0.000181589   -0.000003789
      4        6          -0.000190893   -0.000147838    0.000000155
      5        6           0.000076259    0.000146661   -0.000002731
```

```
      6        6          -0.000037685   -0.000328023    0.000005474
      7        6          -0.000037129    0.000051474    0.000026568
      8        6          -0.000040079    0.000149273   -0.000012855
      9        6           0.000195513    0.000099854    0.000028253
     10        6           0.000128674   -0.000093946   -0.000005892
     11        6          -0.000178582   -0.000064484   -0.000009933
     12        1           0.000055702    0.000002013    0.000006235
     13        6          -0.000110802    0.000259910    0.000008757
     14        6           0.000309072   -0.000129028    0.000002579
     15        6          -0.000248491   -0.000029855   -0.000018508
     16        1           0.000010801   -0.000016629   -0.000034286
     17        1           0.000047316   -0.000053006   -0.000010068
     18        1          -0.000032299   -0.000049774    0.000007071
     19        1           0.000000073   -0.000081941    0.000012734
     20        1           0.000002491    0.000034825    0.000017064
     21        1           0.000023493   -0.000066333   -0.000012619
     22        1          -0.000036589    0.000016408    0.000020730
     23        1          -0.000028777    0.000002340   -0.000004630
     24        6          -0.000014537    0.000065305   -0.000068889
     25        1          -0.000026782    0.000060618   -0.000104433
     26        1           0.000021195   -0.000036354    0.000069477
     27        1           0.000122806    0.000039061    0.000083317
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000328023 RMS     0.000100673


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000326110 RMS     0.000066246
 Search for a local minimum.
 Step number   4 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
 DE= -3.16D-05 DEPred=-2.96D-05 R= 1.07D+00
 SS=  1.41D+00  RLast= 2.70D-02 DXNew= 8.4853D-01 8.0963D-02
 Trust test= 1.07D+00 RLast= 2.70D-02 DXMaxT set to 5.05D-01
     Eigenvalues ---    0.00239   0.01345   0.01742   0.01762
0.01773
     Eigenvalues ---    0.01819   0.01823   0.01904   0.01976
0.01978
     Eigenvalues ---    0.02004   0.02008   0.02031   0.02106
0.02109
     Eigenvalues ---    0.02110   0.02146   0.02147   0.02222
0.02226
     Eigenvalues ---    0.02345   0.02350   0.06755   0.06797
0.12534
     Eigenvalues ---    0.15999   0.15999   0.15999   0.16000
0.16000
```

```
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16005
0.16087
     Eigenvalues ---    0.16451   0.22000   0.22010   0.22402
0.22594
     Eigenvalues ---    0.23502   0.24472   0.24652   0.24998
0.25438
     Eigenvalues ---    0.25745   0.28210   0.33583   0.33615
0.33631
     Eigenvalues ---    0.33646   0.33677   0.33682   0.33682
0.33936
     Eigenvalues ---    0.34367   0.35945   0.36766   0.37237
0.37301
     Eigenvalues ---    0.38355   0.38575   0.39210   0.39512
0.40237
     Eigenvalues ---    0.41160   0.41823   0.44434   0.45020
0.45866
     Eigenvalues ---    0.49621   0.49860   0.50229   0.51349
0.52127
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     4    3
 RFO step:  Lambda=-1.32959832D-06.
 DIIS coeffs:      1.08576     -0.08576
 Iteration  1 RMS(Cart)=  0.00266134 RMS(Int)=  0.00000661
 Iteration  2 RMS(Cart)=  0.00000711 RMS(Int)=  0.00000026
```

This journal is © The Royal Society of Chemistry 2014

```
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000026
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.58920   0.00005   0.00010   0.00011   0.00020
2.58940
    R2        2.69260  -0.00018  -0.00021  -0.00039  -0.00060
2.69200
    R3        2.05389   0.00002   0.00010   0.00001   0.00011
2.05400
    R4        2.70553  -0.00010  -0.00018  -0.00024  -0.00041
2.70511
    R5        2.05584   0.00003   0.00013   0.00001   0.00014
2.05597
    R6        2.73526   0.00013  -0.00006   0.00041   0.00035
2.73560
    R7        2.64191   0.00002  -0.00001   0.00007   0.00006
2.64197
    R8        2.71295   0.00003  -0.00023   0.00008  -0.00015
2.71280
    R9        2.67886   0.00033  -0.00008   0.00073   0.00065
2.67951
   R10        2.59420   0.00016   0.00010   0.00034   0.00044
2.59464
   R11        2.04881  -0.00007   0.00012  -0.00023  -0.00010
2.04871
   R12        2.05443   0.00000   0.00013  -0.00008   0.00005
2.05448
   R13        2.64191   0.00000   0.00000   0.00000   0.00000
2.64191
   R14        2.05696   0.00002   0.00012   0.00000   0.00012
2.05709
   R15        2.67908   0.00007  -0.00005   0.00008   0.00003
2.67911
   R16        2.86215   0.00006  -0.00044   0.00005  -0.00039
2.86176
   R17        2.73551   0.00002  -0.00004   0.00007   0.00003
2.73553
   R18        2.71313  -0.00010  -0.00021  -0.00029  -0.00050
2.71263
   R19        2.70555  -0.00010  -0.00018  -0.00024  -0.00042
2.70513
   R20        2.05584   0.00002   0.00013   0.00001   0.00014
2.05597
   R21        2.58913   0.00009   0.00009   0.00021   0.00030
2.58943
   R22        2.69256  -0.00014  -0.00022  -0.00027  -0.00049
2.69207
   R23        2.05389   0.00002   0.00010   0.00001   0.00011
2.05400
   R24        2.59417   0.00016   0.00010   0.00034   0.00044
2.59462
```

This journal is © The Royal Society of Chemistry 2014

R25	2.05443	0.00000	0.00013	-0.00009	0.00005
2.05448					
R26	2.04869	0.00002	0.00011	0.00005	0.00016
2.04885					
R27	2.07789	-0.00007	-0.00003	-0.00011	-0.00014
2.07775					
R28	2.06451	-0.00005	-0.00006	-0.00001	-0.00007
2.06444					
R29	2.06478	-0.00015	-0.00004	-0.00032	-0.00036
2.06442					
A1	2.08889	0.00004	-0.00005	0.00013	0.00009
2.08898					
A2	2.10344	-0.00009	-0.00010	-0.00054	-0.00063
2.10281					
A3	2.09085	0.00005	0.00014	0.00040	0.00054
2.09139					
A4	2.11630	0.00003	0.00008	0.00008	0.00016
2.11646					
A5	2.10499	-0.00007	-0.00008	-0.00040	-0.00048
2.10451					
A6	2.06189	0.00004	0.00000	0.00032	0.00032
2.06221					
A7	2.08565	-0.00001	-0.00005	-0.00005	-0.00010
2.08555					
A8	2.11125	-0.00002	0.00011	-0.00008	0.00003
2.11128					
A9	2.08628	0.00003	-0.00006	0.00013	0.00007
2.08635					
A10	2.04300	-0.00005	0.00002	-0.00015	-0.00013
2.04286					
A11	2.09323	-0.00009	0.00008	-0.00033	-0.00024
2.09299					
A12	2.14692	0.00014	-0.00010	0.00048	0.00037
2.14729					
A13	2.12461	0.00001	0.00006	0.00009	0.00015
2.12476					
A14	2.08791	0.00004	0.00011	0.00024	0.00035
2.08825					
A15	2.07058	-0.00005	-0.00017	-0.00033	-0.00051
2.07008					
A16	2.10779	-0.00003	-0.00006	-0.00012	-0.00017
2.10761					
A17	2.08556	0.00005	0.00020	0.00032	0.00052
2.08608					
A18	2.08984	-0.00002	-0.00015	-0.00020	-0.00035
2.08949					
A19	2.11889	0.00005	0.00002	0.00012	0.00014
2.11903					
A20	2.08213	-0.00002	-0.00001	-0.00005	-0.00006
2.08207					
A21	2.08211	-0.00003	-0.00001	-0.00007	-0.00007
2.08204					

This journal is © The Royal Society of Chemistry 2014

A22	2.08784	-0.00003	-0.00007	-0.00006	-0.00013
2.08771					
A23	2.09678	0.00030	-0.00002	0.00128	0.00126
2.09804					
A24	2.09842	-0.00026	0.00010	-0.00121	-0.00111
2.09732					
A25	2.09289	0.00005	0.00006	0.00020	0.00026
2.09315					
A26	2.14756	-0.00012	-0.00005	-0.00057	-0.00062
2.14694					
A27	2.04269	0.00007	-0.00001	0.00037	0.00036
2.04306					
A28	2.08647	0.00000	-0.00005	-0.00010	-0.00015
2.08632					
A29	2.11096	0.00006	0.00009	0.00036	0.00045
2.11141					
A30	2.08576	-0.00006	-0.00004	-0.00026	-0.00030
2.08545					
A31	2.06185	0.00004	0.00000	0.00033	0.00034
2.06219					
A32	2.11636	0.00001	0.00008	-0.00001	0.00007
2.11643					
A33	2.10496	-0.00006	-0.00008	-0.00033	-0.00041
2.10455					
A34	2.08882	0.00005	-0.00005	0.00023	0.00018
2.08900					
A35	2.10347	-0.00009	-0.00009	-0.00058	-0.00067
2.10280					
A36	2.09089	0.00004	0.00014	0.00035	0.00049
2.09138					
A37	2.10784	-0.00005	-0.00005	-0.00019	-0.00024
2.10760					
A38	2.08554	0.00007	0.00020	0.00040	0.00059
2.08613					
A39	2.08981	-0.00001	-0.00014	-0.00021	-0.00035
2.08946					
A40	2.12476	-0.00003	0.00007	-0.00015	-0.00008
2.12468					
A41	2.08812	-0.00001	0.00013	-0.00014	-0.00001
2.08811					
A42	2.07022	0.00004	-0.00020	0.00028	0.00008
2.07029					
A43	1.94877	0.00014	0.00050	0.00088	0.00138
1.95016					
A44	1.95307	-0.00008	0.00036	-0.00072	-0.00036
1.95271					
A45	1.95225	0.00003	0.00031	0.00026	0.00057
1.95282					
A46	1.87429	-0.00006	-0.00046	-0.00053	-0.00100
1.87329					
A47	1.87410	-0.00007	-0.00049	-0.00017	-0.00066
1.87345					

This journal is © The Royal Society of Chemistry 2014

A48	1.85620	0.00002	-0.00032	0.00025	-0.00008	1.85612
D1	-0.00141	0.00000	-0.00005	0.00003	-0.00002	-0.00143
D2	3.13518	-0.00001	-0.00005	-0.00034	-0.00039	3.13480
D3	-3.13859	0.00000	-0.00003	0.00014	0.00011	-3.13847
D4	-0.00199	-0.00001	-0.00003	-0.00023	-0.00026	-0.00225
D5	0.00862	0.00001	0.00008	0.00051	0.00059	0.00921
D6	-3.13073	0.00001	0.00013	0.00061	0.00074	-3.12999
D7	-3.13736	0.00001	0.00007	0.00040	0.00046	-3.13690
D8	0.00648	0.00001	0.00012	0.00049	0.00061	0.00709
D9	-0.01211	-0.00001	-0.00007	-0.00055	-0.00062	-0.01273
D10	3.12554	-0.00001	-0.00009	-0.00042	-0.00051	3.12503
D11	3.13436	0.00000	-0.00007	-0.00019	-0.00026	3.13410
D12	-0.01117	0.00000	-0.00009	-0.00006	-0.00015	-0.01132
D13	0.01801	0.00001	0.00015	0.00052	0.00068	0.01869
D14	-3.13265	0.00001	0.00010	0.00026	0.00035	-3.13230
D15	-3.11970	0.00001	0.00017	0.00040	0.00057	-3.11913
D16	0.01283	0.00001	0.00011	0.00013	0.00025	0.01307
D17	-3.12320	0.00001	0.00014	0.00047	0.00061	-3.12259
D18	0.00737	0.00002	0.00012	0.00082	0.00094	0.00831
D19	0.01445	0.00001	0.00012	0.00060	0.00072	0.01517
D20	-3.13816	0.00002	0.00010	0.00095	0.00105	-3.13712
D21	-0.01127	0.00000	-0.00012	0.00000	-0.00012	-0.01140
D22	3.11602	-0.00001	-0.00021	-0.00068	-0.00090	3.11512
D23	3.13969	0.00001	-0.00006	0.00028	0.00022	3.13991
D24	-0.01620	-0.00001	-0.00016	-0.00040	-0.00056	-0.01676
D25	-0.03953	-0.00002	-0.00037	-0.00090	-0.00126	-0.04079

D26	3.12027	-0.00004	-0.00052	-0.00209	-0.00262	3.11765
D27	3.09243	-0.00003	-0.00043	-0.00118	-0.00161	3.09082
D28	-0.03096	-0.00004	-0.00058	-0.00238	-0.00296	-0.03392
D29	-0.00195	-0.00001	0.00000	-0.00052	-0.00052	-0.00246
D30	3.13739	-0.00001	-0.00005	-0.00062	-0.00066	3.13673
D31	-3.12938	0.00000	0.00009	0.00015	0.00024	-3.12913
D32	0.00996	0.00000	0.00004	0.00005	0.00010	0.01006
D33	-0.01450	-0.00001	-0.00010	-0.00055	-0.00065	-0.01514
D34	3.12308	-0.00001	-0.00015	-0.00023	-0.00038	3.12270
D35	3.13812	-0.00002	-0.00008	-0.00090	-0.00098	3.13714
D36	-0.00749	-0.00001	-0.00012	-0.00058	-0.00071	-0.00820
D37	0.03948	0.00002	0.00039	0.00096	0.00134	0.04082
D38	-3.09217	0.00001	0.00049	0.00029	0.00078	-3.09139
D39	-3.12034	0.00004	0.00054	0.00218	0.00272	-3.11761
D40	0.03120	0.00003	0.00065	0.00151	0.00216	0.03336
D41	1.55916	0.00002	0.00032	-0.00559	-0.00527	1.55389
D42	-2.62245	-0.00002	0.00032	-0.00616	-0.00584	-2.62829
D43	-0.54162	-0.00002	0.00037	-0.00616	-0.00579	-0.54741
D44	-1.56412	0.00000	0.00016	-0.00680	-0.00664	-1.57077
D45	0.53746	-0.00003	0.00017	-0.00738	-0.00721	0.53025
D46	2.61829	-0.00003	0.00022	-0.00738	-0.00716	2.61113
D47	-0.01273	-0.00001	-0.00016	-0.00024	-0.00040	-0.01313
D48	3.13282	-0.00001	-0.00011	-0.00056	-0.00067	3.13215
D49	3.11950	0.00000	-0.00026	0.00038	0.00012	3.11963
D50	-0.01813	0.00000	-0.00021	0.00007	-0.00014	-0.01828
D51	-3.13985	0.00000	0.00006	0.00008	0.00015	-3.13970

```
   D52        0.01615   0.00001   0.00017   0.00047   0.00064
0.01679
   D53        0.01143  -0.00001   0.00016  -0.00057  -0.00040
0.01102
   D54       -3.11576   0.00000   0.00028  -0.00018   0.00009  -
3.11567
   D55        0.01122   0.00000   0.00016  -0.00024  -0.00008
0.01113
   D56       -3.12543   0.00000   0.00016  -0.00003   0.00012  -
3.12531
   D57       -3.13439   0.00000   0.00011   0.00008   0.00019  -
3.13420
   D58        0.01215   0.00001   0.00011   0.00028   0.00039
0.01254
   D59        0.00144   0.00000   0.00005  -0.00016  -0.00011
0.00133
   D60        3.13851   0.00000   0.00002   0.00000   0.00001
3.13852
   D61       -3.13509   0.00000   0.00005   0.00005   0.00010  -
3.13499
   D62        0.00198   0.00000   0.00001   0.00021   0.00022
0.00221
   D63       -0.00862  -0.00001  -0.00011  -0.00034  -0.00044  -
0.00906
   D64        3.13070  -0.00001  -0.00016  -0.00033  -0.00049
3.13021
   D65        3.13746  -0.00001  -0.00007  -0.00049  -0.00056
3.13690
   D66       -0.00640  -0.00001  -0.00013  -0.00049  -0.00061  -
0.00701
   D67        0.00185   0.00001  -0.00001   0.00071   0.00071
0.00256
   D68        3.12918   0.00001  -0.00012   0.00033   0.00022
3.12940
   D69       -3.13746   0.00001   0.00005   0.00070   0.00075  -
3.13671
   D70       -0.01013   0.00001  -0.00006   0.00032   0.00026  -
0.00987
         Item               Value     Threshold  Converged?
 Maximum Force            0.000326     0.000450     YES
 RMS     Force            0.000066     0.000300     YES
 Maximum Displacement     0.016503     0.001800     NO
 RMS     Displacement     0.002661     0.001200     NO
 Predicted change in Energy=-1.933108D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

1	6	0	-4.791926	-5.433284	0.004965
2	6	0	-3.422391	-5.398494	-0.022388
3	6	0	-2.710856	-4.156420	-0.033109
4	6	0	-3.449894	-2.911663	-0.030789
5	6	0	-4.882064	-3.002867	0.006306
6	6	0	-5.528447	-4.214078	0.024974
7	6	0	-1.313095	-4.128136	-0.041190
8	6	0	-2.754414	-1.676204	-0.052769
9	6	0	-1.336945	-1.669556	-0.026639
10	6	0	-0.608670	-2.920597	-0.029013
11	6	0	0.822636	-2.902743	-0.014255
12	1	0	1.348045	-3.855397	-0.023448
13	6	0	1.518809	-1.722908	0.016800
14	6	0	0.811431	-0.486518	0.036536
15	6	0	-0.561186	-0.462458	0.014114
16	1	0	-0.761401	-5.066522	-0.047158
17	1	0	-5.319217	-6.383684	0.015746
18	1	0	-2.845365	-6.320799	-0.031557
19	1	0	-5.476597	-2.096731	0.034358
20	1	0	-6.614703	-4.244845	0.057637
21	1	0	2.605648	-1.724225	0.030579
22	1	0	1.366317	0.447727	0.071927
23	1	0	-1.064276	0.497557	0.041824
24	6	0	-3.521153	-0.370600	-0.081818
25	1	0	-3.746157	-0.007913	0.931458
26	1	0	-2.963829	0.417577	-0.593312
27	1	0	-4.471728	-0.468234	-0.611262

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370250	0.000000			
3	C	2.441861	1.431484	0.000000		
4	C	2.856729	2.486998	1.447620	0.000000	
5	C	2.432088	2.805441	2.458939	1.435550	0.000000
6	C	1.424544	2.416724	2.818779	2.453523	1.373023
7	C	3.715886	2.462375	1.398070	2.458826	3.742462
8	C	4.274394	3.781873	2.480676	1.417934	2.508071
9	C	5.109163	4.272479	2.841155	2.451000	3.787700
10	C	4.879998	3.749272	2.438536	2.841239	4.274331
11	C	6.158516	4.924337	3.749350	4.272572	5.705616
12	H	6.339541	5.013802	4.070059	4.889878	6.288239
13	C	7.320683	6.158484	4.880013	5.109150	6.527601
14	C	7.474564	6.485078	5.087193	4.903545	6.224854
15	C	6.527508	5.705460	4.274185	3.787513	5.012357
16	H	4.047514	2.681732	2.151478	3.445531	4.608838
17	H	1.086928	2.137757	3.430254	3.943535	3.408976
18	H	2.139653	1.087975	2.168555	3.462321	3.893359
19	H	3.406203	3.889039	3.449086	2.185379	1.084130
20	H	2.176621	3.395315	3.905903	3.435289	2.132413
21	H	8.275378	7.059767	5.846780	6.171172	7.596140

This journal is © The Royal Society of Chemistry 2014

22	H	8.515559	7.557706	6.150816	5.872984	7.138149
23	H	7.005113	6.350453	4.937240	4.161637	5.179742
24	C	5.220457	5.029215	3.871871	2.542574	2.964570
25	H	5.602381	5.483887	4.383189	3.073346	3.334057
26	H	6.158933	5.861989	4.615113	3.411236	3.967191
27	H	5.013381	5.074972	4.127668	2.711353	2.640858
		6	7	8	9	10
6	C	0.000000				
7	C	4.216747	0.000000			
8	C	3.760600	2.844206	0.000000		
9	C	4.903666	2.458739	1.417725	0.000000	
10	C	5.087260	1.398039	2.480584	1.447582	0.000000
11	C	6.485167	2.462450	3.781689	2.486905	1.431494
12	H	6.886010	2.675139	4.645418	3.462236	2.168551
13	C	7.474611	3.715934	4.274044	2.856582	2.441869
14	C	7.354515	4.216757	3.760130	2.453383	2.818816
15	C	6.224825	3.742409	2.507568	1.435461	2.458976
16	H	4.843200	1.088563	3.932733	3.445438	2.151429
17	H	2.179691	4.597799	5.361277	6.171166	5.846728
18	H	3.411802	2.675017	4.645534	4.889725	4.069912
19	H	2.118003	4.633256	2.755851	4.162081	4.937559
20	H	1.087183	5.303813	4.638097	5.873155	6.150900
21	H	8.506639	4.597879	5.360925	3.943387	3.430262
22	H	8.323005	5.303826	4.637570	3.435146	3.905941
23	H	6.490656	4.633124	2.755131	2.185273	3.449112
24	C	4.337391	4.358468	1.514376	2.541869	3.871412
25	H	4.657263	4.882835	2.176109	3.079499	4.387489
26	H	5.330270	4.867574	2.172547	2.706289	4.124151
27	H	3.943704	4.867938	2.172619	3.407612	4.612625
		11	12	13	14	15
11	C	0.000000				
12	H	1.087974	0.000000			
13	C	1.370267	2.139694	0.000000		
14	C	2.416785	3.411876	1.424582	0.000000	
15	C	2.805488	3.893406	2.432102	1.373012	0.000000
16	H	2.681826	2.432519	4.047616	4.843267	4.608822
17	H	7.059760	7.130649	8.275351	8.506577	7.596037
18	H	5.013745	4.864459	6.339476	6.885901	6.288061
19	H	6.350776	7.047835	7.005409	6.490924	5.180012
20	H	7.557806	7.972678	8.515624	8.323037	7.138166
21	H	2.137767	2.475152	1.086928	2.179717	3.408983
22	H	3.395389	4.304219	2.176683	1.087182	2.132381
23	H	3.889168	4.977124	3.406379	2.118186	1.084203
24	C	5.028401	5.988013	5.219164	4.335750	2.962945
25	H	5.490746	6.454911	5.612279	4.669214	3.345470
26	H	5.069237	6.097156	5.004793	3.932771	2.629852
27	H	5.857776	6.759301	6.152657	5.322757	3.960235
		16	17	18	19	20
16	H	0.000000				
17	H	4.744741	0.000000			
18	H	2.432357	2.475103	0.000000		
19	H	5.573094	4.289881	4.976994	0.000000	

This journal is © The Royal Society of Chemistry 2014

20	H	5.911623	2.500934	4.304120	2.431094	0.000000
21	H	4.744893	9.193165	7.130631	8.090826	9.558720
22	H	5.911709	9.558646	7.972573	7.300764	9.258354
23	H	5.573026	8.090531	7.047527	5.118492	7.300539
24	C	5.446936	6.276921	5.988663	2.610898	4.959766
25	H	5.954492	6.630498	6.449136	2.856987	5.190733
26	H	5.935008	7.223293	6.762789	3.609670	5.957415
27	H	5.935401	6.008655	6.101936	2.019552	4.393468

		21	22	23	24	25
21	H	0.000000				
22	H	2.501005	0.000000			
23	H	4.290080	2.431291	0.000000		
24	C	6.275557	4.957889	2.608683	0.000000	
25	H	6.640989	5.204209	2.870441	1.099498	0.000000
26	H	5.999636	4.381053	2.004519	1.092456	1.765786
27	H	7.216559	5.948824	3.601388	1.092445	1.765880

		26	27
26	H	0.000000	
27	H	1.748926	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.660492	-0.994043	0.021112
2	6	0	-2.462344	-1.658117	-0.011049
3	6	0	-1.219421	-0.948050	-0.020659
4	6	0	-1.225529	0.499532	-0.012019
5	6	0	-2.506248	1.146681	0.029942
6	6	0	-3.677353	0.430159	0.047356
7	6	0	-0.000210	-1.632123	-0.033669
8	6	0	0.000184	1.212083	-0.032850
9	6	0	1.225471	0.499220	-0.011784
10	6	0	1.219116	-0.948322	-0.020458
11	6	0	2.461993	-1.658489	-0.010779
12	1	0	2.432001	-2.745960	-0.024665
13	6	0	3.660192	-0.994467	0.021257
14	6	0	3.677162	0.429777	0.047175
15	6	0	2.506109	1.146360	0.029746
16	1	0	-0.000305	-2.720633	-0.044381
17	1	0	-4.596749	-1.546073	0.030982
18	1	0	-2.432457	-2.745591	-0.025006
19	1	0	-2.559392	2.229009	0.062797
20	1	0	-4.629262	0.954092	0.083824
21	1	0	4.596416	-1.546554	0.031135
22	1	0	4.629092	0.953693	0.083330

This journal is © The Royal Society of Chemistry 2014

```
    23          1          0        2.559100    2.228784    0.062090
    24          6          0        0.000989    2.726292   -0.055300
    25          1          0       -0.007509    3.148563    0.959841
    26          1          0        0.880107    3.125444   -0.566464
    27          1          0       -0.868753    3.126260   -0.581618
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3931793      0.4479189
0.3397588
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8964774208 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860564199     A.U. after   10 cycles
            Convg  =    0.3759D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000034465    0.000016831    0.000004638
      2        6           0.000048573   -0.000028815    0.000002666
      3        6           0.000037772    0.000006585   -0.000009400
      4        6          -0.000040297   -0.000003937    0.000028976
      5        6           0.000015392    0.000084256    0.000004249
      6        6          -0.000032789   -0.000030444   -0.000008127
      7        6           0.000020369   -0.000000255    0.000007300
      8        6          -0.000017838   -0.000084307   -0.000023021
      9        6           0.000052925    0.000024241   -0.000033480
     10        6           0.000006096   -0.000059514   -0.000002959
     11        6           0.000016347   -0.000042315    0.000004162
     12        1           0.000007765    0.000030003    0.000002919
     13        6          -0.000011907    0.000021571    0.000004492
     14        6           0.000029237    0.000021139   -0.000005107
     15        6           0.000075928    0.000090074    0.000030727
     16        1          -0.000013019    0.000016937   -0.000006587
     17        1           0.000016921    0.000005286   -0.000002529
     18        1          -0.000025202    0.000011046    0.000002227
     19        1           0.000037125    0.000078627   -0.000018781
     20        1           0.000024824    0.000001576    0.000004133
     21        1          -0.000012814   -0.000012520   -0.000001711
     22        1          -0.000005343   -0.000024522    0.000001836
     23        1           0.000086833   -0.000066952    0.000013737
     24        6          -0.000129632    0.000170507    0.000002985
     25        1          -0.000007482   -0.000030363    0.000009979
     26        1          -0.000066931   -0.000080553    0.000011246
     27        1          -0.000078392   -0.000114182   -0.000024570
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000170507 RMS     0.000043834


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000501857 RMS     0.000080171
 Search for a local minimum.
```

This journal is © The Royal Society of Chemistry 2014

```
 Step number   5 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
 DE= -5.39D-07 DEPred=-1.93D-06 R= 2.79D-01
 Trust test= 2.79D-01 RLast= 1.75D-02 DXMaxT set to 5.05D-01
     Eigenvalues ---    0.00270   0.01307   0.01569   0.01768
0.01773
     Eigenvalues ---    0.01817   0.01820   0.01832   0.01962
0.01976
     Eigenvalues ---    0.01979   0.02005   0.02023   0.02106
0.02109
     Eigenvalues ---    0.02112   0.02146   0.02146   0.02221
0.02226
     Eigenvalues ---    0.02346   0.02350   0.06792   0.06853
0.11387
     Eigenvalues ---    0.15911   0.15999   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16064
0.16267
     Eigenvalues ---    0.16511   0.21903   0.22001   0.22492
0.22608
     Eigenvalues ---    0.23506   0.24483   0.24629   0.24998
0.25331
     Eigenvalues ---    0.27745   0.32692   0.33583   0.33627
0.33631
     Eigenvalues ---    0.33664   0.33682   0.33682   0.33924
0.34068
     Eigenvalues ---    0.34567   0.36663   0.36944   0.37290
0.37459
     Eigenvalues ---    0.38255   0.38426   0.39432   0.40189
0.40983
     Eigenvalues ---    0.41731   0.42403   0.44428   0.45379
0.49442
     Eigenvalues ---    0.49838   0.49936   0.50633   0.51304
0.57187
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     5    4    3
 RFO step:  Lambda=-1.34120628D-06.
 DIIS coeffs:      0.53872      0.52798     -0.06671
 Iteration  1 RMS(Cart)=  0.00121054 RMS(Int)=  0.00000163
 Iteration  2 RMS(Cart)=  0.00000171 RMS(Int)=  0.00000018
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000018
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.58940   0.00005  -0.00002   0.00009   0.00007
2.58947
    R2        2.69200   0.00002   0.00011  -0.00014  -0.00003
2.69197
    R3        2.05400  -0.00001   0.00003  -0.00003  -0.00001
2.05399
    R4        2.70511   0.00001   0.00005  -0.00009  -0.00004
2.70508
    R5        2.05597  -0.00002   0.00003  -0.00006  -0.00002
2.05595
    R6        2.73560  -0.00006  -0.00021   0.00016  -0.00005
2.73556
    R7        2.64197  -0.00002  -0.00003   0.00001  -0.00002
2.64195
    R8        2.71280  -0.00009  -0.00011   0.00000  -0.00011
2.71268
    R9        2.67951  -0.00017  -0.00036   0.00026  -0.00010
2.67940
   R10        2.59464   0.00002  -0.00012   0.00019   0.00007
2.59471
   R11        2.04871   0.00004   0.00014  -0.00010   0.00005
2.04876
   R12        2.05448  -0.00002   0.00008  -0.00012  -0.00004
2.05444
   R13        2.64191   0.00001   0.00000   0.00002   0.00002
2.64193
   R14        2.05709  -0.00002   0.00004  -0.00006  -0.00002
2.05706
```

R15	2.67911	0.00027	-0.00005	0.00037	0.00031
2.67942					
R16	2.86176	0.00010	-0.00016	0.00034	0.00018
2.86193					
R17	2.73553	0.00013	-0.00005	0.00023	0.00019
2.73572					
R18	2.71263	0.00014	0.00006	0.00007	0.00013
2.71276					
R19	2.70513	0.00001	0.00006	-0.00008	-0.00003
2.70511					
R20	2.05597	-0.00002	0.00003	-0.00006	-0.00002
2.05595					
R21	2.58943	-0.00003	-0.00007	0.00007	0.00000
2.58943					
R22	2.69207	-0.00003	0.00006	-0.00016	-0.00010
2.69197					
R23	2.05400	-0.00001	0.00003	-0.00003	-0.00001
2.05399					
R24	2.59462	0.00001	-0.00013	0.00019	0.00006
2.59468					
R25	2.05448	-0.00002	0.00008	-0.00012	-0.00004
2.05444					
R26	2.04885	-0.00010	0.00001	-0.00014	-0.00013
2.04872					
R27	2.07775	0.00000	0.00004	-0.00007	-0.00003
2.07772					
R28	2.06444	-0.00010	-0.00001	-0.00014	-0.00015
2.06429					
R29	2.06442	0.00009	0.00013	-0.00007	0.00006
2.06448					
A1	2.08898	0.00003	-0.00008	0.00019	0.00011
2.08909					
A2	2.10281	-0.00003	0.00022	-0.00039	-0.00017
2.10264					
A3	2.09139	0.00000	-0.00014	0.00020	0.00006
2.09145					
A4	2.11646	-0.00002	-0.00001	-0.00003	-0.00004
2.11641					
A5	2.10451	0.00000	0.00016	-0.00024	-0.00009
2.10443					
A6	2.06221	0.00003	-0.00014	0.00027	0.00013
2.06233					
A7	2.08555	-0.00006	0.00000	-0.00013	-0.00012
2.08542					
A8	2.11128	0.00008	0.00007	0.00011	0.00019
2.11146					
A9	2.08635	-0.00002	-0.00008	0.00001	-0.00006
2.08629					
A10	2.04286	0.00012	0.00007	0.00016	0.00023
2.04309					
A11	2.09299	0.00010	0.00018	-0.00005	0.00013
2.09312					

This journal is © The Royal Society of Chemistry 2014

A12	2.14729	-0.00022	-0.00025	-0.00011	-0.00036
2.14693					
A13	2.12476	-0.00004	-0.00002	-0.00008	-0.00011
2.12465					
A14	2.08825	-0.00005	-0.00007	-0.00008	-0.00016
2.08810					
A15	2.07008	0.00010	0.00010	0.00016	0.00026
2.07034					
A16	2.10761	-0.00003	0.00004	-0.00011	-0.00007
2.10754					
A17	2.08608	0.00001	-0.00008	0.00016	0.00008
2.08616					
A18	2.08949	0.00001	0.00005	-0.00006	-0.00001
2.08948					
A19	2.11903	0.00001	-0.00005	0.00008	0.00003
2.11905					
A20	2.08207	-0.00001	0.00002	-0.00004	-0.00002
2.08205					
A21	2.08204	0.00000	0.00003	-0.00003	-0.00001
2.08203					
A22	2.08771	0.00000	0.00000	0.00001	0.00001
2.08772					
A23	2.09804	-0.00050	-0.00060	-0.00024	-0.00084
2.09720					
A24	2.09732	0.00050	0.00059	0.00024	0.00083
2.09814					
A25	2.09315	-0.00014	-0.00007	-0.00014	-0.00022
2.09293					
A26	2.14694	0.00023	0.00025	0.00009	0.00033
2.14727					
A27	2.04306	-0.00010	-0.00018	0.00006	-0.00012
2.04294					
A28	2.08632	0.00004	0.00003	0.00006	0.00009
2.08641					
A29	2.11141	-0.00007	-0.00014	0.00003	-0.00011
2.11130					
A30	2.08545	0.00003	0.00011	-0.00009	0.00001
2.08547					
A31	2.06219	0.00002	-0.00015	0.00026	0.00011
2.06230					
A32	2.11643	0.00001	0.00003	-0.00001	0.00002
2.11645					
A33	2.10455	-0.00003	0.00012	-0.00025	-0.00013
2.10442					
A34	2.08900	0.00002	-0.00012	0.00017	0.00005
2.08905					
A35	2.10280	-0.00002	0.00024	-0.00037	-0.00014
2.10266					
A36	2.09138	0.00000	-0.00012	0.00020	0.00009
2.09147					
A37	2.10760	0.00001	0.00007	-0.00009	-0.00002
2.10758					

A38	2.08613	-0.00001	-0.00012	0.00015	0.00003	2.08616
A39	2.08946	0.00000	0.00005	-0.00006	-0.00001	2.08945
A40	2.12468	0.00003	0.00009	-0.00004	0.00005	2.12473
A41	2.08811	0.00003	0.00010	-0.00002	0.00009	2.08820
A42	2.07029	-0.00006	-0.00019	0.00006	-0.00014	2.07016
A43	1.95016	-0.00001	-0.00025	0.00036	0.00011	1.95027
A44	1.95271	0.00005	0.00045	-0.00032	0.00012	1.95283
A45	1.95282	-0.00015	-0.00002	-0.00054	-0.00055	1.95227
A46	1.87329	0.00003	0.00010	0.00010	0.00020	1.87349
A47	1.87345	0.00004	-0.00007	0.00002	-0.00006	1.87339
A48	1.85612	0.00005	-0.00022	0.00041	0.00020	1.85632
D1	-0.00143	0.00000	-0.00003	0.00008	0.00005	-0.00137
D2	3.13480	0.00000	0.00014	-0.00010	0.00004	3.13484
D3	-3.13847	0.00000	-0.00008	0.00004	-0.00004	-3.13851
D4	-0.00225	0.00000	0.00009	-0.00015	-0.00005	-0.00230
D5	0.00921	0.00000	-0.00021	0.00019	-0.00001	0.00920
D6	-3.12999	0.00000	-0.00024	0.00024	0.00001	-3.12998
D7	-3.13690	0.00000	-0.00016	0.00024	0.00008	-3.13682
D8	0.00709	0.00000	-0.00019	0.00029	0.00010	0.00719
D9	-0.01273	0.00000	0.00023	-0.00020	0.00003	-0.01270
D10	3.12503	0.00001	0.00016	-0.00010	0.00006	3.12509
D11	3.13410	0.00000	0.00006	-0.00002	0.00005	3.13415
D12	-0.01132	0.00000	0.00000	0.00008	0.00008	-0.01124
D13	0.01869	-0.00001	-0.00019	0.00005	-0.00014	0.01854
D14	-3.13230	0.00000	-0.00009	0.00020	0.00012	-3.13218
D15	-3.11913	-0.00001	-0.00013	-0.00005	-0.00018	-3.11930

This journal is © The Royal Society of Chemistry 2014

D16	0.01307	0.00000	-0.00002	0.00011	0.00008	0.01316
D17	-3.12259	0.00000	-0.00017	0.00033	0.00016	-3.12243
D18	0.00831	0.00000	-0.00034	0.00051	0.00017	0.00848
D19	0.01517	0.00001	-0.00024	0.00043	0.00019	0.01536
D20	-3.13712	0.00000	-0.00041	0.00061	0.00020	-3.13692
D21	-0.01140	0.00001	-0.00004	0.00023	0.00019	-0.01121
D22	3.11512	0.00001	0.00025	0.00000	0.00024	3.11537
D23	3.13991	-0.00001	-0.00015	0.00006	-0.00008	3.13982
D24	-0.01676	0.00000	0.00014	-0.00016	-0.00003	-0.01679
D25	-0.04079	-0.00001	0.00030	-0.00065	-0.00035	-0.04114
D26	3.11765	-0.00001	0.00080	-0.00128	-0.00048	3.11717
D27	3.09082	0.00000	0.00041	-0.00048	-0.00007	3.09075
D28	-0.03392	0.00000	0.00091	-0.00112	-0.00020	-0.03412
D29	-0.00246	0.00000	0.00024	-0.00035	-0.00011	-0.00258
D30	3.13673	0.00000	0.00027	-0.00040	-0.00013	3.13660
D31	-3.12913	-0.00001	-0.00004	-0.00012	-0.00016	-3.12930
D32	0.01006	-0.00001	-0.00001	-0.00017	-0.00018	0.00988
D33	-0.01514	0.00000	0.00022	-0.00042	-0.00019	-0.01534
D34	3.12270	-0.00001	0.00006	-0.00033	-0.00027	3.12243
D35	3.13714	0.00000	0.00039	-0.00059	-0.00020	3.13694
D36	-0.00820	-0.00001	0.00023	-0.00051	-0.00028	-0.00847
D37	0.04082	0.00001	-0.00032	0.00066	0.00034	0.04116
D38	-3.09139	0.00003	0.00002	0.00067	0.00070	-3.09069
D39	-3.11761	0.00000	-0.00083	0.00129	0.00046	-3.11716
D40	0.03336	0.00002	-0.00049	0.00130	0.00081	0.03417
D41	1.55389	-0.00002	0.00268	0.00027	0.00295	1.55683

D42	-2.62829	0.00004	0.00294	0.00043	0.00337	-2.62492
D43	-0.54741	0.00004	0.00296	0.00037	0.00333	-0.54408
D44	-1.57077	-0.00002	0.00319	-0.00037	0.00282	-1.56794
D45	0.53025	0.00005	0.00346	-0.00021	0.00325	0.53349
D46	2.61113	0.00004	0.00347	-0.00027	0.00320	2.61433
D47	-0.01313	0.00000	0.00006	-0.00014	-0.00007	-0.01320
D48	3.13215	0.00000	0.00022	-0.00022	0.00000	3.13215
D49	3.11963	-0.00002	-0.00026	-0.00015	-0.00041	3.11922
D50	-0.01828	-0.00001	-0.00010	-0.00023	-0.00033	-0.01861
D51	-3.13970	-0.00001	-0.00002	-0.00009	-0.00011	-3.13981
D52	0.01679	0.00000	-0.00016	0.00021	0.00005	0.01684
D53	0.01102	0.00001	0.00031	-0.00008	0.00024	0.01126
D54	-3.11567	0.00002	0.00017	0.00022	0.00040	-3.11527
D55	0.01113	0.00001	0.00016	-0.00001	0.00016	0.01129
D56	-3.12531	0.00001	0.00006	0.00020	0.00027	-3.12504
D57	-3.13420	0.00000	0.00000	0.00008	0.00008	-3.13413
D58	0.01254	0.00000	-0.00010	0.00029	0.00019	0.01273
D59	0.00133	0.00000	0.00009	-0.00003	0.00006	0.00139
D60	3.13852	0.00000	0.00001	-0.00004	-0.00004	3.13849
D61	-3.13499	0.00001	-0.00001	0.00018	0.00017	-3.13482
D62	0.00221	0.00000	-0.00009	0.00017	0.00008	0.00229
D63	-0.00906	0.00000	0.00012	-0.00028	-0.00016	-0.00922
D64	3.13021	-0.00001	0.00010	-0.00036	-0.00026	3.12995
D65	3.13690	0.00000	0.00021	-0.00027	-0.00006	3.13683
D66	-0.00701	0.00000	0.00018	-0.00035	-0.00017	-0.00718
D67	0.00256	-0.00001	-0.00033	0.00033	0.00000	0.00256

```
   D68        3.12940  -0.00001  -0.00019   0.00004  -0.00015
3.12925
   D69       -3.13671   0.00000  -0.00031   0.00042   0.00011  -
3.13660
   D70       -0.00987   0.00000  -0.00017   0.00012  -0.00005  -
0.00992
         Item               Value     Threshold  Converged?
 Maximum Force            0.000502     0.000450     NO
 RMS     Force            0.000080     0.000300     YES
 Maximum Displacement     0.006761     0.001800     NO
 RMS     Displacement     0.001211     0.001200     NO
 Predicted change in Energy=-1.073517D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.791949   -5.432823    0.005085
      2          6           0       -3.422372   -5.398307   -0.022459
      3          6           0       -2.710648   -4.156363   -0.033235
      4          6           0       -3.449629   -2.911600   -0.030730
      5          6           0       -4.881761   -3.002423    0.006407
      6          6           0       -5.528350   -4.213564    0.025173
      7          6           0       -1.312901   -4.128043   -0.041583
      8          6           0       -2.754301   -1.676121   -0.052900
      9          6           0       -1.336668   -1.669304   -0.026713
     10          6           0       -0.608467   -2.920501   -0.029270
     11          6           0        0.822827   -2.902811   -0.014456
     12          1           0        1.348229   -3.855452   -0.023864
     13          6           0        1.519151   -1.723077    0.017046
     14          6           0        0.812017   -0.486616    0.037274
     15          6           0       -0.560626   -0.462329    0.014698
     16          1           0       -0.761211   -5.066415   -0.047878
     17          1           0       -5.319269   -6.383202    0.015869
     18          1           0       -2.845618   -6.320767   -0.031723
     19          1           0       -5.475931   -2.096016    0.034358
     20          1           0       -6.614586   -4.244148    0.057991
     21          1           0        2.605985   -1.724689    0.030892
     22          1           0        1.367024    0.447510    0.073268
     23          1           0       -1.063407    0.497755    0.042944
     24          6           0       -3.522313   -0.371166   -0.082376
     25          1           0       -3.745259   -0.006826    0.930743
     26          1           0       -2.967243    0.416526   -0.596890
     27          1           0       -4.474153   -0.471243   -0.609153
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
```

This journal is © The Royal Society of Chemistry 2014

2	C	1.370288	0.000000			
3	C	2.441849	1.431465	0.000000		
4	C	2.856514	2.486870	1.447596	0.000000	
5	C	2.432059	2.805514	2.459040	1.435489	0.000000
6	C	1.424529	2.416822	2.818888	2.453430	1.373060
7	C	3.715965	2.462479	1.398059	2.458751	3.742470
8	C	4.274129	3.781788	2.480704	1.417879	2.507724
9	C	5.109212	4.272662	2.841359	2.451105	3.787609
10	C	4.880006	3.749351	2.438552	2.841176	4.274228
11	C	6.158494	4.924356	3.749292	4.272496	5.705495
12	H	6.339615	5.013885	4.070027	4.889820	6.288191
13	C	7.320678	6.158533	4.880021	5.109172	6.527519
14	C	7.474652	6.485239	5.087355	4.903753	6.224896
15	C	6.527633	5.705686	4.274433	3.787787	5.012419
16	H	4.047704	2.681899	2.151445	3.445449	4.608898
17	H	1.086924	2.137686	3.430179	3.943317	3.408984
18	H	2.139626	1.087963	2.168609	3.462261	3.893422
19	H	3.406313	3.889146	3.449114	2.185249	1.084155
20	H	2.176638	3.395406	3.905990	3.435187	2.132423
21	H	8.275285	7.059703	5.846687	6.171144	7.596022
22	H	8.515627	7.557847	6.150967	5.873208	7.138194
23	H	7.005370	6.350791	4.937613	4.162113	5.180001
24	C	5.219195	5.028491	3.871554	2.541998	2.963021
25	H	5.603021	5.484607	4.383871	3.074010	3.334611
26	H	6.156850	5.860836	4.614635	3.410228	3.964664
27	H	5.009546	5.072121	4.125741	2.709163	2.636651

		6	7	8	9	10
6	C	0.000000				
7	C	4.216845	0.000000			
8	C	3.760328	2.844237	0.000000		
9	C	4.903687	2.458899	1.417890	0.000000	
10	C	5.087261	1.398047	2.480654	1.447680	0.000000
11	C	6.485144	2.462370	3.781810	2.486988	1.431480
12	H	6.886072	2.675114	4.645544	3.462358	2.168599
13	C	7.474615	3.715887	4.274282	2.856661	2.441870
14	C	7.354627	4.216810	3.760541	2.453506	2.818865
15	C	6.224962	3.742532	2.508000	1.435530	2.459031
16	H	4.843378	1.088551	3.932751	3.445571	2.151423
17	H	2.179709	4.597828	5.361008	6.171203	5.846707
18	H	3.411831	2.675323	4.645592	4.890098	4.070216
19	H	2.118217	4.633111	2.755213	4.161647	4.937208
20	H	1.087162	5.303891	4.637765	5.873109	6.150863
21	H	8.506583	4.597721	5.361161	3.943463	3.430203
22	H	8.323107	5.303855	4.637999	3.435236	3.905967
23	H	6.490960	4.633293	2.755729	2.185331	3.449154
24	C	4.335871	4.358588	1.514470	2.542696	3.872006
25	H	4.657909	4.883259	2.176257	3.079263	4.387550
26	H	5.327661	4.868092	2.172657	2.708240	4.125744
27	H	3.939374	4.867015	2.172335	3.408577	4.612879

		11	12	13	14	15
11	C	0.000000				
12	H	1.087962	0.000000			

This journal is © The Royal Society of Chemistry 2014

```
   13  C    1.370266   2.139605   0.000000
   14  C    2.416772   3.411791   1.424530   0.000000
   15  C    2.805485   3.893392   2.432071   1.373043   0.000000
   16  H    2.681693   2.432436   4.047489   4.843227   4.608878
   17  H    7.059701   7.130682   8.275310   8.506635   7.596145
   18  H    5.014002   4.864791   6.339743   6.886245   6.288453
   19  H    6.350405   7.047564   7.005038   6.490644   5.179723
   20  H    7.557747   7.972716   8.515583   8.323094   7.138239
   21  H    2.137681   2.474894   1.086923   2.179722   3.408994
   22  H    3.395363   4.304099   2.176638   1.087161   2.132387
   23  H    3.889090   4.977034   3.406226   2.118073   1.084135
   24  C    5.029322   5.988811   5.220528   4.337517   2.964679
   25  H    5.490677   6.454984   5.611985   4.668752   3.344922
   26  H    5.071671   6.099299   5.008248   3.937084   2.634052
   27  H    5.858684   6.759849   6.154584   5.325569   3.962948
                 16         17         18         19         20
   16  H    0.000000
   17  H    4.744880   0.000000
   18  H    2.432779   2.474896   0.000000
   19  H    5.573026   4.290088   4.977091   0.000000
   20  H    5.911796   2.501034   4.304127   2.431372   0.000000
   21  H    4.744613   9.193020   7.130767   8.090442   9.558627
   22  H    5.911635   9.558683   7.972888   7.300484   9.258401
   23  H    5.573111   8.090777   7.047985   5.118407   7.300785
   24  C    5.447040   6.275610   5.988174   2.608707   4.958008
   25  H    5.954972   6.631190   6.449926   2.857174   5.191304
   26  H    5.935540   7.221066   6.762050   3.606224   5.954315
   27  H    5.934355   6.004676   6.099383   2.014336   4.388775
                 21         22         23         24         25
   21  H    0.000000
   22  H    2.501053   0.000000
   23  H    4.289970   2.431140   0.000000
   24  C    6.277013   4.959846   2.610929   0.000000
   25  H    6.640714   5.203568   2.869689   1.099481   0.000000
   26  H    6.003314   4.385880   2.010118   1.092377   1.765842
   27  H    7.218666   5.952239   3.605187   1.092478   1.765856
                 26         27
   26  H    0.000000
   27  H    1.749017   0.000000
Stoichiometry    C15H12
Framework group  C1[X(C15H12)]
Deg. of freedom    75
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -3.660196   -0.994409    0.021402
     2          6           0       -2.462015   -1.658489   -0.010988
```

```
      3          6           0       -1.219144   -0.948369   -0.020724
      4          6           0       -1.225502    0.499186   -0.011930
      5          6           0       -2.506129    1.146377    0.030117
      6          6           0       -3.677225    0.429776    0.047696
      7          6           0        0.000215   -1.632149   -0.034039
      8          6           0       -0.000061    1.212088   -0.033019
      9          6           0        1.225603    0.499545   -0.011933
     10          6           0        1.219408   -0.948094   -0.020759
     11          6           0        2.462341   -1.658135   -0.011065
     12          1           0        2.432577   -2.745599   -0.025141
     13          6           0        3.660482   -0.994030    0.021352
     14          6           0        3.677402    0.430155    0.047731
     15          6           0        2.506291    1.146702    0.030183
     16          1           0        0.000351   -2.720644   -0.045056
     17          1           0       -4.596352   -1.546602    0.031328
     18          1           0       -2.432214   -2.745953   -0.025018
     19          1           0       -2.559047    2.228746    0.062849
     20          1           0       -4.629132    0.953655    0.084349
     21          1           0        4.596668   -1.546171    0.031267
     22          1           0        4.629268    0.954104    0.084435
     23          1           0        2.559359    2.229038    0.063037
     24          6           0       -0.001001    2.726384   -0.055925
     25          1           0       -0.006931    3.149059    0.959047
     26          1           0        0.875818    3.126446   -0.570149
     27          1           0       -0.873173    3.124683   -0.579549
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3931292      0.4479101
0.3397526
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8872727227 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
```

```
 Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
           (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860565197     A.U. after    9 cycles
            Convg  =    0.6323D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000002588	-0.000006699	0.000002211
2	6	0.000013780	-0.000025957	0.000003878
3	6	0.000024506	0.000007203	-0.000004147
4	6	-0.000007473	0.000002415	-0.000002962
5	6	-0.000037213	-0.000001668	0.000012999
6	6	-0.000010750	0.000018469	-0.000004767
7	6	0.000005018	-0.000004411	0.000004355
8	6	0.000041997	-0.000049623	-0.000010445
9	6	-0.000008048	0.000011351	-0.000003877
10	6	-0.000022013	-0.000022316	-0.000005148
11	6	0.000017881	-0.000023852	0.000003278
12	1	-0.000001363	0.000016466	0.000001253
13	6	0.000008535	-0.000003590	0.000003300
14	6	-0.000013565	0.000019075	-0.000005775
15	6	0.000020384	0.000027333	0.000011636
16	1	-0.000006507	0.000011384	-0.000000746
17	1	0.000004764	0.000007183	0.000000616

```
     18        1          -0.000014386    0.000008805    0.000000766
     19        1           0.000014936   -0.000005298   -0.000001010
     20        1           0.000010795   -0.000006208   -0.000000026
     21        1          -0.000008603   -0.000000637   -0.000000199
     22        1          -0.000000445   -0.000012223    0.000000178
     23        1          -0.000005225   -0.000013108   -0.000001822
     24        6          -0.000059055    0.000111156    0.000008326
     25        1           0.000009460   -0.000020557    0.000018436
     26        1           0.000026240   -0.000013812   -0.000011168
     27        1          -0.000001061   -0.000030882   -0.000019138
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000111156 RMS     0.000020164


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000052035 RMS     0.000009551
 Search for a local minimum.
 Step number   6 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6
 DE= -9.98D-07 DEPred=-1.07D-06 R= 9.30D-01
 SS=  1.41D+00  RLast= 8.13D-03 DXNew= 8.4853D-01 2.4389D-02
 Trust test= 9.30D-01 RLast= 8.13D-03 DXMaxT set to 5.05D-01
     Eigenvalues ---    0.00279   0.01341   0.01602   0.01769
0.01772
     Eigenvalues ---    0.01819   0.01823   0.01833   0.01956
0.01976
     Eigenvalues ---    0.01978   0.02008   0.02024   0.02106
0.02111
     Eigenvalues ---    0.02111   0.02146   0.02146   0.02222
0.02226
     Eigenvalues ---    0.02347   0.02350   0.06792   0.06863
0.13274
     Eigenvalues ---    0.14853   0.15999   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16004   0.16049
0.16196
     Eigenvalues ---    0.16269   0.21739   0.22001   0.22459
0.22608
     Eigenvalues ---    0.23505   0.24241   0.24484   0.24998
0.25232
     Eigenvalues ---    0.28007   0.32763   0.33585   0.33631
0.33651
     Eigenvalues ---    0.33664   0.33682   0.33682   0.33959
0.34123
```

```
     Eigenvalues ---    0.34558   0.36629   0.36985   0.37299
0.38072
     Eigenvalues ---    0.38251   0.38854   0.39398   0.40184
0.40989
     Eigenvalues ---    0.42068   0.42222   0.44466   0.45386
0.49409
     Eigenvalues ---    0.49760   0.49838   0.50292   0.51317
0.59077
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     6    5    4    3
 RFO step:  Lambda=-3.21999783D-08.
 DIIS coeffs:      1.11499     -0.04780     -0.10022      0.03302
 Iteration  1 RMS(Cart)=  0.00037870 RMS(Int)=  0.00000018
 Iteration  2 RMS(Cart)=  0.00000016 RMS(Int)=  0.00000008
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.58947   0.00000  -0.00001   0.00002   0.00001
2.58948
    R2        2.69197   0.00001   0.00004  -0.00003   0.00001
2.69198
    R3        2.05399  -0.00001  -0.00003   0.00002  -0.00002
2.05397
```

R4	2.70508	0.00001	0.00004	-0.00001	0.00003
2.70511					
R5	2.05595	-0.00002	-0.00004	0.00000	-0.00004
2.05591					
R6	2.73556	0.00001	0.00004	-0.00003	0.00001
2.73557					
R7	2.64195	-0.00001	0.00000	-0.00002	-0.00002
2.64193					
R8	2.71268	0.00002	0.00007	-0.00003	0.00004
2.71272					
R9	2.67940	0.00001	0.00006	-0.00005	0.00001
2.67941					
R10	2.59471	-0.00001	0.00000	-0.00002	-0.00002
2.59469					
R11	2.04876	-0.00001	-0.00005	0.00002	-0.00003
2.04873					
R12	2.05444	-0.00001	-0.00005	0.00003	-0.00002
2.05441					
R13	2.64193	-0.00001	0.00000	-0.00003	-0.00002
2.64190					
R14	2.05706	-0.00001	-0.00004	0.00001	-0.00003
2.05703					
R15	2.67942	-0.00001	0.00006	-0.00005	0.00000
2.67943					
R16	2.86193	0.00005	0.00016	0.00010	0.00026
2.86219					
R17	2.73572	0.00001	0.00004	-0.00001	0.00003
2.73575					
R18	2.71276	0.00001	0.00006	-0.00002	0.00004
2.71280					
R19	2.70511	0.00001	0.00004	0.00000	0.00004
2.70514					
R20	2.05595	-0.00002	-0.00004	0.00000	-0.00004
2.05591					
R21	2.58943	0.00000	-0.00001	0.00002	0.00000
2.58943					
R22	2.69197	0.00001	0.00004	-0.00003	0.00001
2.69198					
R23	2.05399	-0.00001	-0.00003	0.00002	-0.00002
2.05397					
R24	2.59468	-0.00001	0.00000	-0.00002	-0.00003
2.59465					
R25	2.05444	-0.00001	-0.00005	0.00003	-0.00002
2.05441					
R26	2.04872	-0.00001	-0.00005	0.00002	-0.00003
2.04869					
R27	2.07772	0.00001	0.00000	0.00000	0.00000
2.07771					
R28	2.06429	0.00001	0.00000	-0.00001	-0.00001
2.06428					
R29	2.06448	0.00001	0.00000	0.00002	0.00001
2.06450					

This journal is © The Royal Society of Chemistry 2014

A1	2.08909	0.00001	0.00004	0.00002	0.00006
2.08915					
A2	2.10264	-0.00001	-0.00003	-0.00002	-0.00004
2.10260					
A3	2.09145	0.00000	-0.00001	-0.00001	-0.00002
2.09143					
A4	2.11641	0.00000	-0.00002	0.00000	-0.00003
2.11639					
A5	2.10443	-0.00001	-0.00001	-0.00004	-0.00005
2.10438					
A6	2.06233	0.00001	0.00003	0.00004	0.00008
2.06241					
A7	2.08542	-0.00001	0.00000	-0.00004	-0.00004
2.08538					
A8	2.11146	0.00000	-0.00002	0.00005	0.00003
2.11149					
A9	2.08629	0.00000	0.00002	-0.00001	0.00001
2.08630					
A10	2.04309	0.00001	0.00001	0.00005	0.00006
2.04315					
A11	2.09312	-0.00001	-0.00003	0.00000	-0.00003
2.09309					
A12	2.14693	0.00000	0.00002	-0.00005	-0.00003
2.14691					
A13	2.12465	0.00000	-0.00003	0.00000	-0.00003
2.12462					
A14	2.08810	-0.00001	-0.00004	-0.00004	-0.00008
2.08802					
A15	2.07034	0.00001	0.00006	0.00005	0.00011
2.07045					
A16	2.10754	0.00000	0.00000	-0.00002	-0.00002
2.10752					
A17	2.08616	-0.00001	-0.00003	-0.00001	-0.00004
2.08612					
A18	2.08948	0.00001	0.00003	0.00003	0.00006
2.08954					
A19	2.11905	0.00000	0.00001	-0.00001	0.00000
2.11905					
A20	2.08205	0.00000	0.00000	0.00000	0.00000
2.08205					
A21	2.08203	0.00000	0.00000	0.00000	0.00000
2.08203					
A22	2.08772	0.00001	0.00002	0.00002	0.00004
2.08776					
A23	2.09720	0.00000	0.00000	-0.00007	-0.00008
2.09712					
A24	2.09814	0.00000	-0.00002	0.00005	0.00003
2.09818					
A25	2.09293	-0.00001	-0.00003	-0.00002	-0.00005
2.09288					
A26	2.14727	0.00000	0.00002	0.00000	0.00001
2.14728					

```
   A27        2.04294   0.00001   0.00001   0.00003   0.00004
2.04298
   A28        2.08641   0.00001   0.00002   0.00001   0.00003
2.08644
   A29        2.11130   0.00000  -0.00002   0.00003   0.00001
2.11131
   A30        2.08547  -0.00001   0.00000  -0.00003  -0.00004
2.08543
   A31        2.06230   0.00001   0.00003   0.00004   0.00007
2.06237
   A32        2.11645  -0.00001  -0.00002   0.00000  -0.00002
2.11643
   A33        2.10442   0.00000  -0.00001  -0.00004  -0.00005
2.10438
   A34        2.08905   0.00001   0.00004   0.00002   0.00005
2.08910
   A35        2.10266  -0.00001  -0.00002  -0.00001  -0.00004
2.10263
   A36        2.09147   0.00000  -0.00001  -0.00001  -0.00002
2.09145
   A37        2.10758   0.00000   0.00000  -0.00002  -0.00002
2.10756
   A38        2.08616  -0.00001  -0.00003  -0.00001  -0.00004
2.08612
   A39        2.08945   0.00001   0.00003   0.00003   0.00006
2.08950
   A40        2.12473   0.00000  -0.00003   0.00001  -0.00002
2.12471
   A41        2.08820  -0.00001  -0.00004  -0.00003  -0.00007
2.08813
   A42        2.07016   0.00001   0.00007   0.00002   0.00009
2.07025
   A43        1.95027  -0.00002  -0.00009  -0.00006  -0.00015
1.95012
   A44        1.95283  -0.00003  -0.00015  -0.00007  -0.00021
1.95262
   A45        1.95227  -0.00003  -0.00015  -0.00015  -0.00029
1.95197
   A46        1.87349   0.00003   0.00013   0.00013   0.00026
1.87376
   A47        1.87339   0.00003   0.00014   0.00012   0.00025
1.87364
   A48        1.85632   0.00003   0.00014   0.00005   0.00020
1.85652
    D1       -0.00137   0.00000   0.00002  -0.00005  -0.00003  -
0.00140
    D2        3.13484   0.00000   0.00000  -0.00003  -0.00003
3.13480
    D3       -3.13851   0.00000   0.00002  -0.00002  -0.00001  -
3.13852
    D4       -0.00230   0.00000  -0.00001   0.00000  -0.00001  -
0.00231
```

```
    D5        0.00920   0.00000   0.00001  -0.00002  -0.00002
0.00918
    D6       -3.12998   0.00000   0.00000   0.00006   0.00006  -
3.12992
    D7       -3.13682   0.00000   0.00001  -0.00005  -0.00004  -
3.13686
    D8        0.00719   0.00000   0.00001   0.00003   0.00004
0.00722
    D9       -0.01270   0.00000  -0.00001   0.00000  -0.00001  -
0.01271
   D10        3.12509   0.00000   0.00001  -0.00013  -0.00013
3.12497
   D11        3.13415   0.00000   0.00002  -0.00002  -0.00001
3.13414
   D12       -0.01124   0.00000   0.00003  -0.00015  -0.00012  -
0.01136
   D13        0.01854   0.00000  -0.00003   0.00012   0.00009
0.01864
   D14       -3.13218   0.00000   0.00000  -0.00005  -0.00005  -
3.13223
   D15       -3.11930   0.00000  -0.00005   0.00025   0.00021  -
3.11910
   D16        0.01316   0.00000  -0.00002   0.00009   0.00007
0.01322
   D17       -3.12243   0.00000   0.00001   0.00022   0.00022  -
3.12221
   D18        0.00848   0.00000   0.00004   0.00009   0.00013
0.00860
   D19        0.01536   0.00000   0.00002   0.00008   0.00011
0.01547
   D20       -3.13692   0.00000   0.00006  -0.00004   0.00001  -
3.13691
   D21       -0.01121   0.00000   0.00006  -0.00020  -0.00014  -
0.01135
   D22        3.11537   0.00000   0.00005  -0.00012  -0.00007
3.11530
   D23        3.13982   0.00000   0.00003  -0.00003   0.00000
3.13982
   D24       -0.01679   0.00000   0.00002   0.00005   0.00007  -
0.01672
   D25       -0.04114   0.00000   0.00002  -0.00027  -0.00025  -
0.04139
   D26        3.11717   0.00000  -0.00003  -0.00005  -0.00008
3.11709
   D27        3.09075  -0.00001   0.00005  -0.00044  -0.00040
3.09036
   D28       -0.03412   0.00000   0.00000  -0.00022  -0.00022  -
0.03435
   D29       -0.00258   0.00000  -0.00005   0.00016   0.00011  -
0.00247
   D30        3.13660   0.00000  -0.00004   0.00007   0.00003
3.13663
```

This journal is © The Royal Society of Chemistry 2014

D31	-3.12930	0.00000	-0.00004	0.00008	0.00004	-3.12926
D32	0.00988	0.00000	-0.00003	-0.00001	-0.00004	0.00983
D33	-0.01534	0.00000	-0.00003	-0.00007	-0.00010	-0.01543
D34	3.12243	0.00000	0.00000	-0.00021	-0.00021	3.12222
D35	3.13694	0.00000	-0.00006	0.00006	0.00000	3.13694
D36	-0.00847	0.00000	-0.00003	-0.00009	-0.00012	-0.00859
D37	0.04116	0.00000	-0.00002	0.00028	0.00026	0.04142
D38	-3.09069	0.00001	-0.00006	0.00042	0.00037	-3.09033
D39	-3.11716	0.00000	0.00003	0.00006	0.00008	-3.11707
D40	0.03417	0.00000	-0.00001	0.00020	0.00019	0.03437
D41	1.55683	0.00000	-0.00014	-0.00102	-0.00116	1.55567
D42	-2.62492	0.00000	-0.00013	-0.00095	-0.00108	-2.62599
D43	-0.54408	-0.00001	-0.00015	-0.00103	-0.00118	-0.54525
D44	-1.56794	0.00000	-0.00018	-0.00080	-0.00099	-1.56893
D45	0.53349	0.00000	-0.00018	-0.00073	-0.00090	0.53259
D46	2.61433	0.00000	-0.00020	-0.00081	-0.00100	2.61333
D47	-0.01320	0.00000	0.00003	-0.00011	-0.00009	-0.01329
D48	3.13215	0.00000	0.00000	0.00003	0.00003	3.13218
D49	3.11922	0.00000	0.00006	-0.00025	-0.00019	3.11903
D50	-0.01861	0.00000	0.00003	-0.00011	-0.00007	-0.01868
D51	-3.13981	0.00000	-0.00003	0.00005	0.00003	-3.13978
D52	0.01684	0.00000	-0.00002	-0.00003	-0.00005	0.01680
D53	0.01126	0.00000	-0.00006	0.00019	0.00013	0.01139
D54	-3.11527	0.00000	-0.00005	0.00011	0.00006	-3.11521
D55	0.01129	0.00000	-0.00005	0.00016	0.00011	0.01140
D56	-3.12504	0.00000	-0.00002	0.00014	0.00011	-3.12492

```
   D57       -3.13413   0.00000  -0.00002   0.00001  -0.00001  -
3.13414
   D58        0.01273   0.00000   0.00001  -0.00001   0.00000
0.01273
   D59        0.00139   0.00000  -0.00002   0.00005   0.00003
0.00141
   D60        3.13849   0.00000  -0.00001   0.00003   0.00003
3.13851
   D61       -3.13482   0.00000   0.00001   0.00003   0.00003  -
3.13478
   D62        0.00229   0.00000   0.00002   0.00001   0.00003
0.00232
   D63       -0.00922   0.00000  -0.00001   0.00004   0.00003  -
0.00919
   D64        3.12995   0.00000   0.00000  -0.00006  -0.00006
3.12989
   D65        3.13683   0.00000  -0.00002   0.00005   0.00003
3.13687
   D66       -0.00718   0.00000  -0.00001  -0.00005  -0.00006  -
0.00724
   D67        0.00256   0.00000   0.00005  -0.00016  -0.00011
0.00245
   D68        3.12925   0.00000   0.00004  -0.00008  -0.00004
3.12920
   D69       -3.13660   0.00000   0.00004  -0.00007  -0.00002  -
3.13662
   D70       -0.00992   0.00000   0.00003   0.00001   0.00005  -
0.00987
         Item               Value     Threshold  Converged?
 Maximum Force            0.000052     0.000450     YES
 RMS     Force            0.000010     0.000300     YES
 Maximum Displacement     0.002486     0.001800     NO
 RMS     Displacement     0.000379     0.001200     YES
 Predicted change in Energy=-4.813161D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.791961   -5.432750    0.005313
      2          6           0       -3.422383   -5.398310   -0.022488
      3          6           0       -2.710619   -4.156372   -0.033453
      4          6           0       -3.449617   -2.911611   -0.030878
      5          6           0       -4.881765   -3.002368    0.006636
      6          6           0       -5.528367   -4.213490    0.025519
      7          6           0       -1.312883   -4.128050   -0.041914
      8          6           0       -2.754265   -1.676142   -0.053178
      9          6           0       -1.336633   -1.669289   -0.026880
```

10	6	0	-0.608456	-2.920519	-0.029520
11	6	0	0.822855	-2.902816	-0.014559
12	1	0	1.348326	-3.855396	-0.024020
13	6	0	1.519138	-1.723062	0.017157
14	6	0	0.812024	-0.486584	0.037496
15	6	0	-0.560604	-0.462288	0.014852
16	1	0	-0.761199	-5.066406	-0.048272
17	1	0	-5.319289	-6.383114	0.016232
18	1	0	-2.845738	-6.320813	-0.031812
19	1	0	-5.475806	-2.095900	0.034714
20	1	0	-6.614580	-4.244124	0.058599
21	1	0	2.605963	-1.724678	0.031089
22	1	0	1.367079	0.447490	0.073714
23	1	0	-1.063463	0.497733	0.043223
24	6	0	-3.522423	-0.371115	-0.082684
25	1	0	-3.746261	-0.007455	0.930480
26	1	0	-2.966802	0.416713	-0.596379
27	1	0	-4.473702	-0.471299	-0.610468

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370292	0.000000			
3	C	2.441849	1.431482	0.000000		
4	C	2.856455	2.486862	1.447603	0.000000	
5	C	2.432040	2.805562	2.459107	1.435510	0.000000
6	C	1.424534	2.416872	2.818943	2.453419	1.373049
7	C	3.715973	2.462505	1.398049	2.458756	3.742517
8	C	4.274076	3.781780	2.480693	1.417885	2.507730
9	C	5.109204	4.272701	2.841384	2.451139	3.787636
10	C	4.879982	3.749358	2.438532	2.841176	4.274246
11	C	6.158500	4.924389	3.749293	4.272513	5.705528
12	H	6.339718	5.014006	4.070099	4.889891	6.288293
13	C	7.320648	6.158544	4.880000	5.109158	6.527503
14	C	7.474640	6.485281	5.087376	4.903776	6.224898
15	C	6.527630	5.705742	4.274476	3.787832	5.012435
16	H	4.047730	2.681926	2.151423	3.445437	4.608940
17	H	1.086916	2.137659	3.430161	3.943250	3.408953
18	H	2.139583	1.087942	2.168656	3.462273	3.893451
19	H	3.406328	3.889181	3.449123	2.185206	1.084139
20	H	2.176605	3.395414	3.906032	3.435198	2.132441
21	H	8.275249	7.059703	5.846653	6.171119	7.595996
22	H	8.515613	7.557882	6.150988	5.873250	7.138212
23	H	7.005266	6.350760	4.937580	4.162073	5.179911
24	C	5.219158	5.028551	3.871643	2.542067	2.962985
25	H	5.602075	5.484010	4.383518	3.073488	3.333521
26	H	6.157065	5.861007	4.614718	3.410373	3.964950
27	H	5.009637	5.072123	4.125672	2.709206	2.636977

		6	7	8	9	10
6	C	0.000000				
7	C	4.216889	0.000000			
8	C	3.760315	2.844216	0.000000		

This journal is © The Royal Society of Chemistry 2014

9	C	4.903706	2.458922	1.417892	0.000000	
10	C	5.087271	1.398035	2.480631	1.447697	0.000000
11	C	6.485175	2.462382	3.781800	2.486992	1.431499
12	H	6.886188	2.675199	4.645562	3.462380	2.168644
13	C	7.474599	3.715885	4.274240	2.856617	2.441872
14	C	7.354626	4.216849	3.760544	2.453500	2.818918
15	C	6.224973	3.742587	2.508030	1.435553	2.459097
16	H	4.843428	1.088534	3.932713	3.445575	2.151398
17	H	2.179695	4.597824	5.360947	6.171187	5.846674
18	H	3.411832	2.675436	4.645622	4.890205	4.070312
19	H	2.118262	4.633081	2.755124	4.161556	4.937127
20	H	1.087149	5.303920	4.637786	5.873143	6.150872
21	H	8.506558	4.597704	5.361110	3.943411	3.430189
22	H	8.323114	5.303879	4.638037	3.435248	3.906006
23	H	6.490862	4.633285	2.755691	2.185296	3.449170
24	C	4.335823	4.358703	1.514606	2.542843	3.872144
25	H	4.656778	4.883255	2.176270	3.079697	4.387865
26	H	5.327959	4.868034	2.172621	2.707985	4.125560
27	H	3.939643	4.866813	2.172253	3.408366	4.612625

		11	12	13	14	15
11	C	0.000000				
12	H	1.087942	0.000000			
13	C	1.370268	2.139561	0.000000		
14	C	2.416817	3.411788	1.424536	0.000000	
15	C	2.805530	3.893418	2.432054	1.373030	0.000000
16	H	2.681695	2.432536	4.047489	4.843260	4.608918
17	H	7.059700	7.130783	8.275275	8.506616	7.596134
18	H	5.014139	4.865030	6.339863	6.886383	6.288588
19	H	6.350329	7.047556	7.004896	6.490510	5.179603
20	H	7.557771	7.972816	8.515565	8.323101	7.138264
21	H	2.137654	2.474803	1.086915	2.179710	3.408965
22	H	3.395368	4.304037	2.176607	1.087148	2.132398
23	H	3.889122	4.977045	3.406235	2.118104	1.084118
24	C	5.029473	5.988978	5.220639	4.337650	2.964827
25	H	5.491178	6.455426	5.612655	4.669576	3.345692
26	H	5.071419	6.099085	5.007867	3.936658	2.633635
27	H	5.858405	6.759589	6.154264	5.325316	3.962757

		16	17	18	19	20
16	H	0.000000				
17	H	4.744898	0.000000			
18	H	2.432923	2.474801	0.000000		
19	H	5.572998	4.290109	4.977105	0.000000	
20	H	5.911821	2.500970	4.304065	2.431510	0.000000
21	H	4.744600	9.192979	7.130882	8.090291	9.558597
22	H	5.911641	9.558659	7.973011	7.300372	9.258420
23	H	5.573094	8.090663	7.048029	5.118181	7.300708
24	C	5.447137	6.275559	5.988272	2.608519	4.957983
25	H	5.954958	6.630180	6.449453	2.855753	5.190067
26	H	5.935461	7.221297	6.762223	3.606467	5.954719
27	H	5.934118	6.004775	6.099338	2.014895	4.389216

		21	22	23	24	25
21	H	0.000000				

```
   22  H    2.500993   0.000000
   23  H    4.289982   2.431252   0.000000
   24  C    6.277117   4.960021   2.610984   0.000000
   25  H    6.641423   5.204542   2.870513   1.099479   0.000000
   26  H    6.002915   4.385487   2.009566   1.092369   1.766005
   27  H    7.218325   5.952058   3.605006   1.092485   1.766024
                 26         27
   26  H    0.000000
   27  H    1.749146   0.000000
 Stoichiometry    C15H12
 Framework group  C1[X(C15H12)]
 Deg. of freedom    75
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.660166   -0.994396    0.021606
      2          6           0       -2.462015   -1.658527   -0.011018
      3          6           0       -1.219120   -0.948417   -0.020929
      4          6           0       -1.225512    0.499145   -0.012074
      5          6           0       -2.506127    1.146384    0.030324
      6          6           0       -3.677215    0.429792    0.048008
      7          6           0        0.000239   -1.632174   -0.034332
      8          6           0       -0.000064    1.212042   -0.033279
      9          6           0        1.225627    0.499545   -0.012058
     10          6           0        1.219411   -0.948111   -0.020957
     11          6           0        2.462374   -1.658135   -0.011090
     12          1           0        2.432714   -2.745581   -0.025213
     13          6           0        3.660482   -0.993977    0.021554
     14          6           0        3.677411    0.430212    0.048034
     15          6           0        2.506308    1.146744    0.030396
     16          1           0        0.000389   -2.720652   -0.045404
     17          1           0       -4.596314   -1.546584    0.031655
     18          1           0       -2.432317   -2.745973   -0.025100
     19          1           0       -2.558917    2.228739    0.063176
     20          1           0       -4.629135    0.953604    0.084903
     21          1           0        4.596665   -1.546107    0.031574
     22          1           0        4.629285    0.954103    0.084975
     23          1           0        2.559264    2.229066    0.063369
     24          6           0       -0.001111    2.726474   -0.056225
     25          1           0       -0.008176    3.149020    0.958791
     26          1           0        0.876256    3.126378   -0.569619
     27          1           0       -0.872852    3.124386   -0.580874
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3930947      0.4479086
0.3397511
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
```

This journal is © The Royal Society of Chemistry 2014

```
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8832643546 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860565261     A.U. after    8 cycles
             Convg  =    0.7643D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
```

This journal is © The Royal Society of Chemistry 2014

```
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000000279   -0.000006424   -0.000000146
      2        6           0.000001675   -0.000002017   -0.000000675
      3        6          -0.000002168    0.000000059    0.000000730
      4        6           0.000001023    0.000002244    0.000003824
      5        6          -0.000003286    0.000000269   -0.000004707
      6        6          -0.000001956    0.000007471    0.000001961
      7        6           0.000003698   -0.000000380    0.000002093
      8        6           0.000015287   -0.000003016    0.000008670
      9        6          -0.000014051    0.000004079   -0.000001922
     10        6          -0.000001954   -0.000004970    0.000000878
     11        6           0.000003604   -0.000001011   -0.000000879
     12        1          -0.000000972    0.000001676    0.000000987
     13        6           0.000006744   -0.000006570   -0.000000345
     14        6          -0.000008986    0.000006487    0.000002018
     15        6           0.000007643    0.000000058   -0.000004937
     16        1          -0.000000607    0.000001551   -0.000000395
     17        1           0.000000401    0.000002329    0.000000858
     18        1          -0.000001544    0.000001357    0.000000921
     19        1           0.000002028    0.000001871   -0.000000527
     20        1           0.000001878   -0.000001332    0.000000304
     21        1          -0.000002268    0.000000665    0.000000786
     22        1          -0.000000108   -0.000002170    0.000000083
     23        1           0.000000311   -0.000000431   -0.000000316
     24        6           0.000000003    0.000009481    0.000000276
     25        1          -0.000000772   -0.000004984    0.000002837
     26        1           0.000000052   -0.000000352   -0.000001299
     27        1          -0.000005953   -0.000005940   -0.000011077
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000015287 RMS     0.000004202


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000016873 RMS     0.000003019
 Search for a local minimum.
 Step number   7 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7
 DE= -6.36D-08 DEPred=-4.81D-08 R= 1.32D+00
 Trust test= 1.32D+00 RLast= 2.85D-03 DXMaxT set to 5.05D-01
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.00192   0.01351   0.01604   0.01769
0.01787
     Eigenvalues ---    0.01814   0.01819   0.01833   0.01967
0.01976
     Eigenvalues ---    0.01978   0.02024   0.02040   0.02106
0.02111
     Eigenvalues ---    0.02138   0.02146   0.02167   0.02226
0.02233
     Eigenvalues ---    0.02347   0.02374   0.06751   0.06864
0.12658
     Eigenvalues ---    0.15194   0.15995   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16005   0.16055
0.16212
     Eigenvalues ---    0.16450   0.21905   0.22002   0.22533
0.22608
     Eigenvalues ---    0.23534   0.24416   0.24543   0.24998
0.25236
     Eigenvalues ---    0.28227   0.32669   0.33586   0.33631
0.33659
     Eigenvalues ---    0.33673   0.33682   0.33682   0.33956
0.34066
     Eigenvalues ---    0.34485   0.36653   0.36982   0.37274
0.38087
     Eigenvalues ---    0.38302   0.38687   0.39442   0.40185
0.40981
     Eigenvalues ---    0.41610   0.42366   0.44592   0.45386
0.49688
     Eigenvalues ---    0.49834   0.49959   0.51311   0.52032
0.58805
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     7    6    5    4
3
 RFO step:  Lambda= 0.00000000D+00.
 DIIS coeffs:      1.16255     -0.10259     -0.02793     -0.04047
0.00844
 Iteration  1 RMS(Cart)=  0.00042775 RMS(Int)=  0.00000027
 Iteration  2 RMS(Cart)=  0.00000028 RMS(Int)=  0.00000002
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.58948   0.00000   0.00000   0.00001   0.00001
2.58949
    R2        2.69198   0.00000   0.00000   0.00000   0.00000
2.69198
    R3        2.05397   0.00000  -0.00001   0.00000  -0.00001
2.05396
    R4        2.70511   0.00000   0.00001   0.00000   0.00000
2.70511
    R5        2.05591   0.00000  -0.00002   0.00000  -0.00002
2.05590
    R6        2.73557   0.00000   0.00002  -0.00002   0.00000
2.73557
    R7        2.64193   0.00000   0.00000   0.00000   0.00000
2.64193
    R8        2.71272   0.00000   0.00002  -0.00002   0.00000
2.71272
    R9        2.67941  -0.00001   0.00002  -0.00003  -0.00001
2.67941
   R10        2.59469   0.00000   0.00000  -0.00001   0.00000
2.59469
   R11        2.04873   0.00000  -0.00002   0.00001  -0.00001
2.04872
   R12        2.05441   0.00000  -0.00002   0.00001  -0.00001
2.05440
   R13        2.64190   0.00000   0.00000  -0.00001  -0.00001
2.64190
   R14        2.05703   0.00000  -0.00001   0.00000  -0.00001
2.05702
   R15        2.67943  -0.00001   0.00003  -0.00003  -0.00001
2.67942
   R16        2.86219   0.00000   0.00008   0.00001   0.00009
2.86228
   R17        2.73575   0.00001   0.00002   0.00002   0.00004
2.73579
```

This journal is © The Royal Society of Chemistry 2014

R18	2.71280	0.00000	0.00002	0.00000	0.00002
2.71282					
R19	2.70514	0.00000	0.00001	0.00000	0.00001
2.70515					
R20	2.05591	0.00000	-0.00002	0.00000	-0.00002
2.05590					
R21	2.58943	0.00000	0.00000	0.00000	0.00000
2.58943					
R22	2.69198	0.00001	0.00000	0.00000	0.00001
2.69199					
R23	2.05397	0.00000	-0.00001	0.00000	-0.00001
2.05396					
R24	2.59465	0.00000	0.00000	-0.00001	-0.00001
2.59464					
R25	2.05441	0.00000	-0.00002	0.00001	-0.00001
2.05440					
R26	2.04869	0.00000	-0.00002	0.00000	-0.00001
2.04867					
R27	2.07771	0.00000	0.00000	0.00000	0.00000
2.07771					
R28	2.06428	0.00000	-0.00001	-0.00001	-0.00001
2.06426					
R29	2.06450	0.00001	0.00000	0.00004	0.00003
2.06453					
A1	2.08915	0.00000	0.00002	0.00000	0.00003
2.08918					
A2	2.10260	0.00000	-0.00003	0.00000	-0.00003
2.10257					
A3	2.09143	0.00000	0.00000	-0.00001	0.00000
2.09143					
A4	2.11639	0.00000	-0.00001	0.00000	-0.00001
2.11638					
A5	2.10438	0.00000	-0.00002	-0.00001	-0.00003
2.10435					
A6	2.06241	0.00000	0.00003	0.00001	0.00004
2.06245					
A7	2.08538	0.00000	-0.00001	-0.00001	-0.00002
2.08536					
A8	2.11149	0.00000	0.00001	0.00003	0.00004
2.11153					
A9	2.08630	0.00000	0.00001	-0.00002	-0.00001
2.08629					
A10	2.04315	0.00000	0.00002	0.00002	0.00004
2.04319					
A11	2.09309	0.00000	-0.00001	0.00002	0.00001
2.09310					
A12	2.14691	-0.00001	0.00000	-0.00004	-0.00005
2.14686					
A13	2.12462	0.00000	-0.00001	-0.00001	-0.00002
2.12461					
A14	2.08802	0.00000	-0.00002	-0.00002	-0.00004
2.08798					

This journal is © The Royal Society of Chemistry 2014

A15	2.07045	0.00000	0.00003	0.00003	0.00006
2.07051					
A16	2.10752	0.00000	-0.00001	-0.00001	-0.00001
2.10751					
A17	2.08612	0.00000	-0.00001	-0.00001	-0.00001
2.08610					
A18	2.08954	0.00000	0.00001	0.00001	0.00003
2.08957					
A19	2.11905	0.00000	0.00000	0.00000	0.00000
2.11905					
A20	2.08205	0.00000	0.00000	0.00000	0.00000
2.08205					
A21	2.08203	0.00000	0.00000	0.00000	0.00000
2.08203					
A22	2.08776	0.00000	0.00001	0.00001	0.00002
2.08778					
A23	2.09712	-0.00002	-0.00002	-0.00010	-0.00012
2.09700					
A24	2.09818	0.00001	0.00001	0.00010	0.00011
2.09828					
A25	2.09288	0.00000	-0.00002	-0.00002	-0.00004
2.09284					
A26	2.14728	0.00000	0.00001	0.00003	0.00003
2.14732					
A27	2.04298	0.00000	0.00001	-0.00001	0.00000
2.04299					
A28	2.08644	0.00000	0.00001	0.00001	0.00002
2.08646					
A29	2.11131	0.00000	0.00000	-0.00001	0.00000
2.11131					
A30	2.08543	0.00000	-0.00001	0.00000	-0.00001
2.08542					
A31	2.06237	0.00000	0.00003	0.00000	0.00003
2.06240					
A32	2.11643	0.00000	-0.00001	0.00000	0.00000
2.11643					
A33	2.10438	0.00000	-0.00002	-0.00001	-0.00003
2.10435					
A34	2.08910	0.00000	0.00002	-0.00001	0.00002
2.08912					
A35	2.10263	0.00000	-0.00003	0.00001	-0.00002
2.10261					
A36	2.09145	0.00000	0.00000	0.00000	0.00000
2.09145					
A37	2.10756	0.00000	-0.00001	0.00000	0.00000
2.10756					
A38	2.08612	0.00000	-0.00001	-0.00001	-0.00001
2.08610					
A39	2.08950	0.00000	0.00001	0.00000	0.00002
2.08952					
A40	2.12471	0.00000	-0.00001	0.00001	0.00000
2.12471					

This journal is © The Royal Society of Chemistry 2014

A41	2.08813	0.00000	-0.00002	0.00000	-0.00002	2.08811
A42	2.07025	0.00000	0.00003	-0.00001	0.00002	2.07026
A43	1.95012	-0.00001	-0.00002	-0.00003	-0.00005	1.95006
A44	1.95262	0.00000	-0.00007	0.00004	-0.00003	1.95258
A45	1.95197	-0.00001	-0.00009	-0.00008	-0.00018	1.95180
A46	1.87376	0.00000	0.00007	0.00005	0.00012	1.87388
A47	1.87364	0.00001	0.00006	0.00003	0.00010	1.87374
A48	1.85652	0.00000	0.00007	-0.00001	0.00007	1.85658
D1	-0.00140	0.00000	0.00000	0.00002	0.00002	-0.00138
D2	3.13480	0.00000	-0.00001	0.00001	0.00000	3.13480
D3	-3.13852	0.00000	0.00000	0.00002	0.00003	-3.13849
D4	-0.00231	0.00000	-0.00001	0.00001	0.00000	-0.00231
D5	0.00918	0.00000	0.00001	0.00002	0.00003	0.00921
D6	-3.12992	0.00000	0.00002	0.00001	0.00003	-3.12989
D7	-3.13686	0.00000	0.00001	0.00002	0.00003	-3.13684
D8	0.00722	0.00000	0.00002	0.00001	0.00003	0.00726
D9	-0.01271	0.00000	-0.00001	-0.00003	-0.00005	-0.01276
D10	3.12497	0.00000	-0.00002	-0.00002	-0.00004	3.12493
D11	3.13414	0.00000	0.00000	-0.00002	-0.00002	3.13412
D12	-0.01136	0.00000	-0.00001	0.00000	-0.00001	-0.01138
D13	0.01864	0.00000	0.00001	0.00000	0.00002	0.01865
D14	-3.13223	0.00000	0.00000	0.00002	0.00003	-3.13220
D15	-3.11910	0.00000	0.00002	-0.00001	0.00001	-3.11909
D16	0.01322	0.00000	0.00001	0.00001	0.00002	0.01324
D17	-3.12221	0.00000	0.00005	-0.00001	0.00004	-3.12217
D18	0.00860	0.00000	0.00005	0.00003	0.00008	0.00868

D19	0.01547	0.00000	0.00004	0.00001	0.00005	0.01552
D20	-3.13691	0.00000	0.00004	0.00005	0.00008	-3.13682
D21	-0.01135	0.00000	0.00000	0.00004	0.00003	-0.01132
D22	3.11530	0.00000	0.00000	-0.00002	-0.00002	3.11528
D23	3.13982	0.00000	0.00001	0.00002	0.00002	3.13985
D24	-0.01672	0.00000	0.00001	-0.00004	-0.00003	-0.01675
D25	-0.04139	0.00000	-0.00007	-0.00003	-0.00009	-0.04149
D26	3.11709	0.00000	-0.00007	-0.00018	-0.00025	3.11684
D27	3.09036	0.00000	-0.00008	-0.00001	-0.00008	3.09027
D28	-0.03435	0.00000	-0.00009	-0.00016	-0.00024	-0.03459
D29	-0.00247	0.00000	-0.00001	-0.00005	-0.00006	-0.00253
D30	3.13663	0.00000	-0.00002	-0.00004	-0.00006	3.13656
D31	-3.12926	0.00000	0.00000	0.00000	0.00000	-3.12926
D32	0.00983	0.00000	-0.00002	0.00001	-0.00001	0.00983
D33	-0.01543	0.00000	-0.00004	0.00000	-0.00004	-0.01547
D34	3.12222	0.00000	-0.00005	0.00001	-0.00004	3.12218
D35	3.13694	0.00000	-0.00004	-0.00004	-0.00008	3.13686
D36	-0.00859	0.00000	-0.00005	-0.00003	-0.00007	-0.00867
D37	0.04142	0.00000	0.00007	0.00003	0.00010	0.04152
D38	-3.09033	0.00000	0.00008	0.00001	0.00009	-3.09024
D39	-3.11707	0.00000	0.00007	0.00018	0.00026	-3.11681
D40	0.03437	0.00000	0.00009	0.00016	0.00025	0.03461
D41	1.55567	0.00000	-0.00021	-0.00118	-0.00139	1.55428
D42	-2.62599	0.00000	-0.00019	-0.00110	-0.00129	-2.62729
D43	-0.54525	0.00000	-0.00021	-0.00114	-0.00136	-0.54661
D44	-1.56893	-0.00001	-0.00022	-0.00133	-0.00155	-1.57048

This journal is © The Royal Society of Chemistry 2014

D45	0.53259	0.00000	-0.00020	-0.00125	-0.00145	0.53114
D46	2.61333	0.00000	-0.00022	-0.00129	-0.00151	2.61182
D47	-0.01329	0.00000	-0.00002	-0.00002	-0.00003	-0.01333
D48	3.13218	0.00000	-0.00001	-0.00003	-0.00004	3.13215
D49	3.11903	0.00000	-0.00003	0.00000	-0.00002	3.11901
D50	-0.01868	0.00000	-0.00002	-0.00001	-0.00003	-0.01871
D51	-3.13978	0.00000	0.00000	-0.00001	-0.00001	-3.13979
D52	0.01680	0.00000	0.00000	0.00005	0.00005	0.01685
D53	0.01139	0.00000	0.00001	-0.00003	-0.00002	0.01137
D54	-3.11521	0.00000	0.00001	0.00003	0.00004	-3.11517
D55	0.01140	0.00000	0.00001	0.00001	0.00001	0.01141
D56	-3.12492	0.00000	0.00002	0.00002	0.00005	-3.12488
D57	-3.13414	0.00000	0.00000	0.00002	0.00002	-3.13412
D58	0.01273	0.00000	0.00001	0.00004	0.00005	0.01278
D59	0.00141	0.00000	0.00000	-0.00002	-0.00002	0.00139
D60	3.13851	0.00000	0.00000	-0.00002	-0.00002	3.13849
D61	-3.13478	0.00000	0.00001	0.00000	0.00001	-3.13477
D62	0.00232	0.00000	0.00002	-0.00001	0.00001	0.00233
D63	-0.00919	0.00000	-0.00001	-0.00002	-0.00003	-0.00922
D64	3.12989	0.00000	-0.00003	-0.00002	-0.00004	3.12985
D65	3.13687	0.00000	-0.00001	-0.00002	-0.00003	3.13684
D66	-0.00724	0.00000	-0.00003	-0.00001	-0.00004	-0.00728
D67	0.00245	0.00000	0.00001	0.00005	0.00005	0.00250
D68	3.12920	0.00000	0.00000	-0.00001	-0.00001	3.12919
D69	-3.13662	0.00000	0.00002	0.00004	0.00006	-3.13656
D70	-0.00987	0.00000	0.00002	-0.00002	0.00000	-0.00987

```
         Item               Value     Threshold  Converged?
 Maximum Force            0.000017     0.000450     YES
 RMS     Force            0.000003     0.000300     YES
 Maximum Displacement     0.002931     0.001800     NO
 RMS     Displacement     0.000428     0.001200     YES
 Predicted change in Energy=-1.771381D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.791976   -5.432670    0.005452
      2          6           0       -3.422393   -5.398291   -0.022490
      3          6           0       -2.710588   -4.156373   -0.033467
      4          6           0       -3.449575   -2.911606   -0.030809
      5          6           0       -4.881723   -3.002294    0.006817
      6          6           0       -5.528359   -4.213395    0.025768
      7          6           0       -1.312854   -4.128049   -0.042023
      8          6           0       -2.754225   -1.676141   -0.053150
      9          6           0       -1.336596   -1.669261   -0.026860
     10          6           0       -0.608430   -2.920521   -0.029591
     11          6           0        0.822887   -2.902822   -0.014683
     12          1           0        1.348381   -3.855379   -0.024228
     13          6           0        1.519172   -1.723070    0.017123
     14          6           0        0.812075   -0.486580    0.037588
     15          6           0       -0.560547   -0.462266    0.014940
     16          1           0       -0.761170   -5.066395   -0.048524
     17          1           0       -5.319319   -6.383020    0.016402
     18          1           0       -2.845821   -6.320829   -0.031896
     19          1           0       -5.475678   -2.095776    0.034979
     20          1           0       -6.614561   -4.244025    0.058990
     21          1           0        2.605992   -1.724707    0.031034
     22          1           0        1.367153    0.447468    0.073917
     23          1           0       -1.063408    0.497742    0.043419
     24          6           0       -3.522567   -0.371170   -0.082901
     25          1           0       -3.747777   -0.008196    0.930205
     26          1           0       -2.966400    0.416991   -0.595475
     27          1           0       -4.473121   -0.471380   -0.612019
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1          2          3          4          5
    1  C    0.000000
    2  C    1.370299   0.000000
    3  C    2.441848   1.431484   0.000000
    4  C    2.856417   2.486847   1.447603   0.000000
    5  C    2.432032   2.805584   2.459136   1.435510   0.000000
    6  C    1.424536   2.416898   2.818971   2.453406   1.373048
    7  C    3.715990   2.462530   1.398047   2.458747   3.742531
```

This journal is © The Royal Society of Chemistry 2014

8	C	4.274035	3.781770	2.480694	1.417880	2.507694
9	C	5.109201	4.272731	2.841412	2.451146	3.787617
10	C	4.879977	3.749371	2.438527	2.841159	4.274231
11	C	6.158508	4.924412	3.749292	4.272502	5.705519
12	H	6.339772	5.014066	4.070124	4.889900	6.288316
13	C	7.320646	6.158562	4.879999	5.109144	6.527479
14	C	7.474639	6.485309	5.087395	4.903783	6.224878
15	C	6.527633	5.705778	4.274511	3.787854	5.012422
16	H	4.047773	2.681966	2.151417	3.445424	4.608962
17	H	1.086911	2.137646	3.430148	3.943207	3.408942
18	H	2.139565	1.087934	2.168677	3.462271	3.893465
19	H	3.406344	3.889201	3.449126	2.185177	1.084136
20	H	2.176594	3.395424	3.906052	3.435192	2.132450
21	H	8.275238	7.059710	5.846638	6.171097	7.595966
22	H	8.515608	7.557906	6.151004	5.873262	7.138194
23	H	7.005244	6.350776	4.937601	4.162086	5.179877
24	C	5.219002	5.028481	3.871629	2.542018	2.962797
25	H	5.600932	5.483304	4.383127	3.072827	3.332133
26	H	6.157303	5.861207	4.614863	3.410552	3.965190
27	H	5.009724	5.072083	4.125582	2.709272	2.637317

		6	7	8	9	10
6	C	0.000000				
7	C	4.216914	0.000000			
8	C	3.760280	2.844209	0.000000		
9	C	4.903699	2.458949	1.417890	0.000000	
10	C	5.087267	1.398031	2.480619	1.447716	0.000000
11	C	6.485181	2.462380	3.781793	2.487004	1.431505
12	H	6.886234	2.675226	4.645567	3.462401	2.168663
13	C	7.474589	3.715883	4.274232	2.856613	2.441876
14	C	7.354617	4.216865	3.760557	2.453503	2.818939
15	C	6.224969	3.742616	2.508057	1.435561	2.459124
16	H	4.843472	1.088527	3.932698	3.445592	2.151387
17	H	2.179692	4.597833	5.360900	6.171181	5.846665
18	H	3.411834	2.675514	4.645640	4.890283	4.070383
19	H	2.118295	4.633051	2.755025	4.161458	4.937051
20	H	1.087142	5.303938	4.637758	5.873133	6.150863
21	H	8.506542	4.597688	5.361098	3.943402	3.430183
22	H	8.323103	5.303888	4.638062	3.435252	3.906020
23	H	6.490833	4.633299	2.755714	2.185286	3.449182
24	C	4.335632	4.358742	1.514656	2.542960	3.872237
25	H	4.655339	4.883366	2.176275	3.080406	4.388433
26	H	5.328232	4.868050	2.172633	2.707772	4.125437
27	H	3.939921	4.866560	2.172185	3.408096	4.612304

		11	12	13	14	15
11	C	0.000000				
12	H	1.087933	0.000000			
13	C	1.370270	2.139538	0.000000		
14	C	2.416832	3.411782	1.424539	0.000000	
15	C	2.805546	3.893425	2.432049	1.373025	0.000000
16	H	2.681684	2.432561	4.047480	4.843266	4.608935
17	H	7.059705	7.130837	8.275269	8.506612	7.596133
18	H	5.014229	4.865165	6.339949	6.886472	6.288675

This journal is © The Royal Society of Chemistry 2014

19	H	6.350253	7.047516	7.004794	6.490405	5.179504
20	H	7.557770	7.972855	8.515549	8.323087	7.138258
21	H	2.137640	2.474754	1.086910	2.179710	3.408957
22	H	3.395368	4.304008	2.176596	1.087141	2.132398
23	H	3.889129	4.977044	3.406232	2.118103	1.084110
24	C	5.029601	5.989097	5.220801	4.337852	2.965034
25	H	5.492053	6.456205	5.613845	4.670960	3.346987
26	H	5.071211	6.098918	5.007543	3.936252	2.633215
27	H	5.858023	6.759204	6.153870	5.324991	3.962498

		16	17	18	19	20
16	H	0.000000				
17	H	4.744938	0.000000			
18	H	2.433033	2.474751	0.000000		
19	H	5.572982	4.290134	4.977117	0.000000	
20	H	5.911856	2.500953	4.304042	2.431585	0.000000
21	H	4.744575	9.192967	7.130958	8.090184	9.558574
22	H	5.911636	9.558649	7.973092	7.300269	9.258406
23	H	5.573098	8.090636	7.048091	5.118059	7.300678
24	C	5.447167	6.275389	5.988240	2.608218	4.957778
25	H	5.955091	6.628964	6.448914	2.853956	5.188422
26	H	5.935463	7.221549	6.762424	3.606653	5.955038
27	H	5.933824	6.004868	6.099238	2.015536	4.389632

		21	22	23	24	25
21	H	0.000000				
22	H	2.500981	0.000000			
23	H	4.289980	2.431272	0.000000		
24	C	6.277282	4.960253	2.611212	0.000000	
25	H	6.642687	5.206089	2.871968	1.099479	0.000000
26	H	6.002577	4.385053	2.009001	1.092361	1.766078
27	H	7.217907	5.951772	3.604850	1.092503	1.766103

		26	27
26	H	0.000000	
27	H	1.749196	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.660130	-0.994418	0.021661
2	6	0	-2.461988	-1.658573	-0.011072
3	6	0	-1.219087	-0.948470	-0.020974
4	6	0	-1.225503	0.499091	-0.012052
5	6	0	-2.506101	1.146357	0.030424
6	6	0	-3.677190	0.429769	0.048157
7	6	0	0.000290	-1.632191	-0.034439
8	6	0	-0.000077	1.212018	-0.033278

```
      9          6           0        1.225643    0.499577   -0.012031
     10          6           0        1.219440   -0.948098   -0.021006
     11          6           0        2.462424   -1.658098   -0.011158
     12          1           0        2.432823   -2.745536   -0.025354
     13          6           0        3.660515   -0.993910    0.021597
     14          6           0        3.677428    0.430280    0.048188
     15          6           0        2.506321    1.146795    0.030512
     16          1           0        0.000474   -2.720661   -0.045642
     17          1           0       -4.596270   -1.546611    0.031726
     18          1           0       -2.432342   -2.746011   -0.025223
     19          1           0       -2.558819    2.228710    0.063347
     20          1           0       -4.629112    0.953555    0.085169
     21          1           0        4.596696   -1.546031    0.031622
     22          1           0        4.629294    0.954162    0.085254
     23          1           0        2.559240    2.229108    0.063583
     24          6           0       -0.001349    2.726495   -0.056484
     25          1           0       -0.009978    3.149156    0.958472
     26          1           0        0.876660    3.126422   -0.568743
     27          1           0       -0.872480    3.123996   -0.582494
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3930849      0.4479082
0.3397510
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8820721269 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860565287     A.U. after    7 cycles
            Convg  =    0.8243D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000004214   -0.000003843   -0.000000574
      2        6          -0.000005748    0.000005785    0.000000703
      3        6          -0.000012859    0.000001473    0.000002180
      4        6           0.000005589   -0.000003819    0.000003878
      5        6           0.000006838   -0.000000392   -0.000002748
      6        6           0.000002832    0.000003064    0.000001209
      7        6           0.000003290    0.000001899   -0.000001002
      8        6           0.000007073    0.000016173   -0.000000631
      9        6          -0.000014068   -0.000002161   -0.000003055
     10        6           0.000001748    0.000003039    0.000002043
     11        6           0.000000964    0.000009721    0.000000720
     12        1          -0.000001386   -0.000004905    0.000000797
     13        6           0.000002758   -0.000009502   -0.000000901
     14        6          -0.000008268    0.000000544    0.000001189
     15        6           0.000005342   -0.000009337   -0.000002983
     16        1           0.000001846   -0.000002530    0.000001895
     17        1          -0.000002577   -0.000000240    0.000000898
     18        1           0.000004318   -0.000001509    0.000000947
     19        1          -0.000002892    0.000003919   -0.000000652
     20        1          -0.000002804    0.000000121   -0.000000591
     21        1           0.000001423    0.000001943    0.000000990
     22        1           0.000000855    0.000002627   -0.000000847
     23        1           0.000002158    0.000004672   -0.000000327
```

```
     24        6           0.000021771   -0.000026110    0.000001304
     25        1          -0.000006106    0.000002658   -0.000004690
     26        1          -0.000010845    0.000003045    0.000005976
     27        1          -0.000005467    0.000003665   -0.000005729
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000026110 RMS     0.000006042


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000021048 RMS     0.000004066
 Search for a local minimum.
 Step number   8 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8
 DE= -2.60D-08 DEPred=-1.77D-08 R= 1.47D+00
 Trust test= 1.47D+00 RLast= 3.57D-03 DXMaxT set to 5.05D-01
     Eigenvalues ---    0.00034   0.01481   0.01707   0.01769
0.01791
     Eigenvalues ---    0.01819   0.01829   0.01900   0.01971
0.01976
     Eigenvalues ---    0.01988   0.02024   0.02049   0.02106
0.02111
     Eigenvalues ---    0.02145   0.02146   0.02182   0.02226
0.02246
     Eigenvalues ---    0.02347   0.02427   0.06790   0.06869
0.13790
     Eigenvalues ---    0.15769   0.15956   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16003   0.16018   0.16193
0.16212
     Eigenvalues ---    0.19916   0.21996   0.22123   0.22608
0.22672
     Eigenvalues ---    0.23535   0.24457   0.24944   0.25003
0.26469
     Eigenvalues ---    0.28231   0.32263   0.33586   0.33631
0.33661
     Eigenvalues ---    0.33682   0.33682   0.33691   0.33961
0.34032
     Eigenvalues ---    0.35279   0.36961   0.37211   0.37325
0.38063
     Eigenvalues ---    0.38304   0.39376   0.39546   0.40280
0.40967
     Eigenvalues ---    0.41295   0.44418   0.45385   0.47090
0.49665
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.49835   0.50424   0.51296   0.51906
0.62767
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     8    7    6    5
4
 RFO step:  Lambda= 0.00000000D+00.
 DIIS coeffs:      1.44017      0.26157     -0.62846     -0.03855
-0.03473
 Iteration  1 RMS(Cart)=  0.00143171 RMS(Int)=  0.00000311
 Iteration  2 RMS(Cart)=  0.00000323 RMS(Int)=  0.00000002
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000002
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.58949   0.00000   0.00002   0.00002   0.00005
2.58954
    R2        2.69198   0.00000  -0.00001   0.00002   0.00001
2.69199
    R3        2.05396   0.00000  -0.00001  -0.00002  -0.00003
2.05394
    R4        2.70511   0.00000   0.00001   0.00000   0.00000
2.70512
    R5        2.05590   0.00000  -0.00003  -0.00002  -0.00005
2.05585
```

This journal is © The Royal Society of Chemistry 2014

R6	2.73557	-0.00001	0.00002	-0.00003	-0.00001
2.73556					
R7	2.64193	0.00000	-0.00001	0.00001	-0.00001
2.64192					
R8	2.71272	0.00000	0.00001	-0.00003	-0.00002
2.71270					
R9	2.67941	-0.00001	0.00002	-0.00005	-0.00003
2.67937					
R10	2.59469	0.00000	0.00001	0.00000	0.00000
2.59469					
R11	2.04872	0.00000	-0.00002	0.00001	-0.00001
2.04871					
R12	2.05440	0.00000	-0.00002	-0.00001	-0.00004
2.05436					
R13	2.64190	0.00000	-0.00002	0.00000	-0.00002
2.64187					
R14	2.05702	0.00000	-0.00003	-0.00001	-0.00004
2.05698					
R15	2.67942	-0.00001	0.00002	-0.00005	-0.00002
2.67940					
R16	2.86228	-0.00001	0.00022	0.00001	0.00024
2.86252					
R17	2.73579	0.00000	0.00005	0.00006	0.00012
2.73591					
R18	2.71282	0.00000	0.00003	0.00001	0.00004
2.71286					
R19	2.70515	0.00000	0.00001	0.00001	0.00003
2.70518					
R20	2.05590	0.00000	-0.00003	-0.00002	-0.00005
2.05585					
R21	2.58943	0.00000	0.00001	0.00000	0.00001
2.58945					
R22	2.69199	0.00000	-0.00001	0.00002	0.00001
2.69200					
R23	2.05396	0.00000	-0.00001	-0.00002	-0.00003
2.05393					
R24	2.59464	0.00000	0.00000	-0.00002	-0.00003
2.59462					
R25	2.05440	0.00000	-0.00002	-0.00001	-0.00004
2.05436					
R26	2.04867	0.00000	-0.00003	-0.00001	-0.00004
2.04863					
R27	2.07771	0.00000	-0.00001	0.00002	0.00001
2.07772					
R28	2.06426	-0.00001	-0.00003	-0.00002	-0.00005
2.06422					
R29	2.06453	0.00001	0.00002	0.00010	0.00012
2.06465					
A1	2.08918	0.00000	0.00006	0.00001	0.00008
2.08926					
A2	2.10257	0.00000	-0.00007	-0.00001	-0.00008
2.10249					

A3	2.09143	0.00000	0.00001	-0.00001	0.00000
2.09143					
A4	2.11638	0.00000	-0.00002	-0.00001	-0.00003
2.11634					
A5	2.10435	0.00000	-0.00007	-0.00001	-0.00008
2.10426					
A6	2.06245	0.00000	0.00009	0.00003	0.00012
2.06257					
A7	2.08536	0.00000	-0.00005	-0.00002	-0.00007
2.08529					
A8	2.11153	0.00000	0.00005	0.00007	0.00012
2.11165					
A9	2.08629	0.00000	0.00000	-0.00004	-0.00004
2.08625					
A10	2.04319	0.00000	0.00007	0.00006	0.00013
2.04332					
A11	2.09310	0.00001	-0.00002	0.00006	0.00004
2.09314					
A12	2.14686	-0.00001	-0.00005	-0.00012	-0.00017
2.14669					
A13	2.12461	0.00000	-0.00003	-0.00003	-0.00006
2.12455					
A14	2.08798	0.00000	-0.00007	-0.00005	-0.00012
2.08786					
A15	2.07051	0.00000	0.00010	0.00007	0.00018
2.07068					
A16	2.10751	0.00000	-0.00003	-0.00001	-0.00004
2.10747					
A17	2.08610	0.00000	-0.00001	-0.00001	-0.00003
2.08608					
A18	2.08957	0.00000	0.00004	0.00002	0.00007
2.08964					
A19	2.11905	0.00000	0.00001	-0.00001	0.00000
2.11905					
A20	2.08205	0.00000	0.00000	0.00001	0.00001
2.08206					
A21	2.08203	0.00000	0.00000	0.00000	-0.00001
2.08202					
A22	2.08778	0.00000	0.00003	0.00002	0.00005
2.08783					
A23	2.09700	-0.00002	-0.00012	-0.00028	-0.00041
2.09659					
A24	2.09828	0.00002	0.00009	0.00027	0.00037
2.09865					
A25	2.09284	0.00000	-0.00006	-0.00005	-0.00011
2.09273					
A26	2.14732	0.00001	0.00003	0.00008	0.00011
2.14742					
A27	2.04299	-0.00001	0.00004	-0.00003	0.00001
2.04300					
A28	2.08646	0.00000	0.00003	0.00003	0.00006
2.08651					

```
   A29        2.11131   0.00000   0.00001  -0.00003  -0.00002
2.11129
   A30        2.08542   0.00000  -0.00004   0.00000  -0.00004
2.08538
   A31        2.06240   0.00000   0.00008   0.00000   0.00009
2.06249
   A32        2.11643   0.00000  -0.00001   0.00001   0.00000
2.11642
   A33        2.10435   0.00000  -0.00007  -0.00001  -0.00008
2.10426
   A34        2.08912   0.00000   0.00005  -0.00002   0.00004
2.08915
   A35        2.10261   0.00000  -0.00007   0.00001  -0.00006
2.10255
   A36        2.09145   0.00000   0.00001   0.00001   0.00002
2.09147
   A37        2.10756   0.00000  -0.00002   0.00001  -0.00001
2.10755
   A38        2.08610   0.00000  -0.00001  -0.00001  -0.00003
2.08608
   A39        2.08952   0.00000   0.00003   0.00000   0.00003
2.08955
   A40        2.12471   0.00000  -0.00001   0.00002   0.00000
2.12472
   A41        2.08811   0.00000  -0.00005   0.00001  -0.00004
2.08807
   A42        2.07026  -0.00001   0.00006  -0.00003   0.00003
2.07030
   A43        1.95006   0.00000  -0.00007  -0.00005  -0.00012
1.94994
   A44        1.95258   0.00001  -0.00017   0.00011  -0.00006
1.95252
   A45        1.95180   0.00000  -0.00031  -0.00024  -0.00054
1.95125
   A46        1.87388  -0.00001   0.00022   0.00012   0.00034
1.87422
   A47        1.87374  -0.00001   0.00019   0.00006   0.00026
1.87400
   A48        1.85658  -0.00001   0.00018   0.00001   0.00018
1.85677
    D1       -0.00138   0.00000  -0.00001   0.00005   0.00004  -
0.00134
    D2        3.13480   0.00000  -0.00004   0.00001  -0.00002
3.13478
    D3       -3.13849   0.00000   0.00001   0.00005   0.00006  -
3.13844
    D4       -0.00231   0.00000  -0.00002   0.00002   0.00000  -
0.00232
    D5        0.00921   0.00000   0.00002   0.00006   0.00008
0.00928
    D6       -3.12989   0.00000   0.00008   0.00003   0.00011  -
3.12978
```

This journal is © The Royal Society of Chemistry 2014

D7	-3.13684	0.00000	0.00000	0.00006	0.00006	-3.13678
D8	0.00726	0.00000	0.00007	0.00003	0.00010	0.00735
D9	-0.01276	0.00000	-0.00005	-0.00007	-0.00012	-0.01287
D10	3.12493	0.00000	-0.00012	-0.00002	-0.00013	3.12479
D11	3.13412	0.00000	-0.00002	-0.00004	-0.00006	3.13407
D12	-0.01138	0.00000	-0.00009	0.00002	-0.00008	-0.01145
D13	0.01865	0.00000	0.00008	0.00000	0.00008	0.01873
D14	-3.13220	0.00000	0.00000	0.00006	0.00006	-3.13214
D15	-3.11909	0.00000	0.00016	-0.00006	0.00010	-3.11899
D16	0.01324	0.00000	0.00007	0.00000	0.00007	0.01332
D17	-3.12217	0.00000	0.00021	-0.00002	0.00019	-3.12198
D18	0.00868	0.00000	0.00017	0.00007	0.00024	0.00892
D19	0.01552	0.00000	0.00013	0.00004	0.00017	0.01569
D20	-3.13682	0.00000	0.00010	0.00013	0.00022	-3.13660
D21	-0.01132	0.00000	-0.00007	0.00011	0.00003	-0.01128
D22	3.11528	0.00000	-0.00007	-0.00001	-0.00009	3.11519
D23	3.13985	0.00000	0.00001	0.00004	0.00006	3.13990
D24	-0.01675	0.00000	0.00002	-0.00008	-0.00006	-0.01681
D25	-0.04149	0.00000	-0.00029	-0.00005	-0.00034	-0.04183
D26	3.11684	0.00000	-0.00029	-0.00035	-0.00064	3.11620
D27	3.09027	0.00000	-0.00038	0.00001	-0.00036	3.08991
D28	-0.03459	0.00000	-0.00038	-0.00028	-0.00066	-0.03525
D29	-0.00253	0.00000	0.00002	-0.00014	-0.00011	-0.00264
D30	3.13656	0.00000	-0.00004	-0.00011	-0.00015	3.13642
D31	-3.12926	0.00000	0.00002	-0.00002	0.00001	-3.12926
D32	0.00983	0.00000	-0.00004	0.00001	-0.00003	0.00980

This journal is © The Royal Society of Chemistry 2014

D33	-0.01547	0.00000	-0.00012	-0.00002	-0.00015	-0.01562
D34	3.12218	0.00000	-0.00020	0.00003	-0.00017	3.12201
D35	3.13686	0.00000	-0.00008	-0.00011	-0.00020	3.13666
D36	-0.00867	0.00000	-0.00016	-0.00006	-0.00023	-0.00889
D37	0.04152	0.00000	0.00030	0.00006	0.00036	0.04188
D38	-3.09024	0.00000	0.00038	0.00001	0.00038	-3.08985
D39	-3.11681	0.00000	0.00030	0.00035	0.00066	-3.11616
D40	0.03461	0.00000	0.00038	0.00030	0.00068	0.03529
D41	1.55428	-0.00001	-0.00139	-0.00343	-0.00483	1.54945
D42	-2.62729	0.00000	-0.00128	-0.00324	-0.00452	-2.63181
D43	-0.54661	0.00000	-0.00138	-0.00332	-0.00470	-0.55131
D44	-1.57048	0.00000	-0.00140	-0.00373	-0.00513	-1.57561
D45	0.53114	0.00000	-0.00129	-0.00353	-0.00482	0.52632
D46	2.61182	0.00000	-0.00138	-0.00361	-0.00500	2.60682
D47	-0.01333	0.00000	-0.00010	-0.00003	-0.00012	-0.01345
D48	3.13215	0.00000	-0.00002	-0.00008	-0.00010	3.13205
D49	3.11901	0.00000	-0.00017	0.00003	-0.00014	3.11886
D50	-0.01871	0.00000	-0.00009	-0.00002	-0.00012	-0.01882
D51	-3.13979	0.00000	0.00001	-0.00002	-0.00001	-3.13981
D52	0.01685	0.00000	0.00002	0.00012	0.00013	0.01698
D53	0.01137	0.00000	0.00009	-0.00008	0.00001	0.01138
D54	-3.11517	0.00000	0.00009	0.00006	0.00015	-3.11502
D55	0.01141	0.00000	0.00009	-0.00001	0.00008	0.01149
D56	-3.12488	0.00000	0.00012	0.00003	0.00016	-3.12472
D57	-3.13412	0.00000	0.00001	0.00004	0.00005	-3.13407
D58	0.01278	0.00000	0.00005	0.00008	0.00013	0.01291

```
   D59        0.00139   0.00000   0.00001  -0.00004  -0.00003
0.00136
   D60        3.13849   0.00000   0.00001  -0.00005  -0.00005
3.13844
   D61       -3.13477   0.00000   0.00005   0.00000   0.00005  -
3.13472
   D62        0.00233   0.00000   0.00004  -0.00001   0.00003
0.00236
   D63       -0.00922   0.00000  -0.00002  -0.00007  -0.00009  -
0.00930
   D64        3.12985   0.00000  -0.00010  -0.00004  -0.00014
3.12971
   D65        3.13684   0.00000  -0.00001  -0.00005  -0.00007
3.13677
   D66       -0.00728   0.00000  -0.00009  -0.00003  -0.00012  -
0.00740
   D67        0.00250   0.00000  -0.00003   0.00013   0.00009
0.00259
   D68        3.12919   0.00000  -0.00004  -0.00001  -0.00005
3.12914
   D69       -3.13656   0.00000   0.00005   0.00010   0.00015  -
3.13642
   D70       -0.00987   0.00000   0.00004  -0.00004   0.00000  -
0.00987
         Item               Value     Threshold  Converged?
 Maximum Force            0.000021     0.000450     YES
 RMS     Force            0.000004     0.000300     YES
 Maximum Displacement     0.009626     0.001800     NO
 RMS     Displacement     0.001432     0.001200     NO
 Predicted change in Energy=-5.163169D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792027   -5.432402    0.005936
      2          6           0       -3.422425   -5.398220   -0.022461
      3          6           0       -2.710483   -4.156380   -0.033556
      4          6           0       -3.449421   -2.911590   -0.030678
      5          6           0       -4.881565   -3.002041    0.007379
      6          6           0       -5.528322   -4.213074    0.026567
      7          6           0       -1.312754   -4.128044   -0.042416
      8          6           0       -2.754091   -1.676137   -0.053202
      9          6           0       -1.336474   -1.669174   -0.026895
     10          6           0       -0.608342   -2.920525   -0.029877
     11          6           0        0.822992   -2.902846   -0.015072
     12          1           0        1.348545   -3.855339   -0.024855
     13          6           0        1.519289   -1.723101    0.017020
```

14	6	0	0.812247	-0.486580	0.037860
15	6	0	-0.560361	-0.462206	0.015188
16	1	0	-0.761069	-5.066364	-0.049293
17	1	0	-5.319422	-6.382705	0.017021
18	1	0	-2.846081	-6.320870	-0.032089
19	1	0	-5.475245	-2.095359	0.035793
20	1	0	-6.614492	-4.243659	0.060253
21	1	0	2.606094	-1.724811	0.030892
22	1	0	1.367380	0.447399	0.074542
23	1	0	-1.063208	0.497775	0.044006
24	6	0	-3.523038	-0.371392	-0.083559
25	1	0	-3.752859	-0.010810	0.929370
26	1	0	-2.965113	0.418008	-0.592247
27	1	0	-4.471184	-0.471565	-0.617113

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370323	0.000000			
3	C	2.441847	1.431485	0.000000		
4	C	2.856295	2.486790	1.447598	0.000000	
5	C	2.432010	2.805647	2.459221	1.435501	0.000000
6	C	1.424541	2.416977	2.819050	2.453358	1.373049
7	C	3.716050	2.462611	1.398045	2.458708	3.742562
8	C	4.273898	3.781735	2.480704	1.417863	2.507556
9	C	5.109189	4.272820	2.841503	2.451155	3.787529
10	C	4.879962	3.749412	2.438514	2.841094	4.274163
11	C	6.158533	4.924481	3.749285	4.272451	5.705463
12	H	6.339929	5.014244	4.070186	4.889906	6.288357
13	C	7.320638	6.158619	4.879998	5.109096	6.527381
14	C	7.474628	6.485391	5.087452	4.903793	6.224786
15	C	6.527628	5.705880	4.274614	3.787909	5.012347
16	H	4.047920	2.682100	2.151403	3.445379	4.609026
17	H	1.086896	2.137608	3.430108	3.943072	3.408914
18	H	2.139516	1.087910	2.168734	3.462255	3.893504
19	H	3.406396	3.889261	3.449134	2.185089	1.084129
20	H	2.176565	3.395459	3.906110	3.435163	2.132475
21	H	8.275207	7.059732	5.846595	6.171021	7.595848
22	H	8.515577	7.557969	6.151051	5.873283	7.138099
23	H	7.005179	6.350833	4.937681	4.162134	5.179759
24	C	5.218444	5.028206	3.871547	2.541814	2.962124
25	H	5.596986	5.480817	4.381726	3.070552	3.327387
26	H	6.158144	5.861937	4.615409	3.411179	3.965990
27	H	5.010093	5.072025	4.125344	2.709544	2.638506

		6	7	8	9	10
6	C	0.000000				
7	C	4.216990	0.000000			
8	C	3.760156	2.844190	0.000000		
9	C	4.903659	2.459033	1.417878	0.000000	
10	C	5.087246	1.398019	2.480581	1.447779	0.000000
11	C	6.485184	2.462371	3.781771	2.487042	1.431519
12	H	6.886358	2.675293	4.645573	3.462463	2.168712

13	C	7.474548	3.715878	4.274215	2.856609	2.441892
14	C	7.354570	4.216911	3.760599	2.453512	2.818998
15	C	6.224932	3.742698	2.508138	1.435582	2.459200
16	H	4.843610	1.088507	3.932657	3.445648	2.151355
17	H	2.179685	4.597870	5.360749	6.171156	5.846637
18	H	3.411841	2.675758	4.645692	4.890523	4.070605
19	H	2.118400	4.632953	2.754696	4.161129	4.936797
20	H	1.087122	5.303992	4.637644	5.873078	6.150825
21	H	8.506480	4.597638	5.361065	3.943384	3.430163
22	H	8.323041	5.303911	4.638129	3.435258	3.906058
23	H	6.490735	4.633352	2.755799	2.185262	3.449223
24	C	4.334952	4.358839	1.514780	2.543327	3.872520
25	H	4.650413	4.883656	2.176304	3.082780	4.390283
26	H	5.329155	4.868182	2.172682	2.707105	4.125098
27	H	3.940908	4.865778	2.171958	3.407204	4.611269

		11	12	13	14	15
11	C	0.000000				
12	H	1.087909	0.000000			
13	C	1.370276	2.139473	0.000000		
14	C	2.416870	3.411758	1.424545	0.000000	
15	C	2.805585	3.893441	2.432037	1.373012	0.000000
16	H	2.681647	2.432622	4.047448	4.843278	4.608982
17	H	7.059723	7.130997	8.275256	8.506591	7.596115
18	H	5.014506	4.865571	6.340216	6.886741	6.288934
19	H	6.349993	7.047363	7.004458	6.490049	5.179160
20	H	7.557752	7.972954	8.515484	8.323016	7.138201
21	H	2.137600	2.474608	1.086895	2.179714	3.408938
22	H	3.395369	4.303927	2.176570	1.087122	2.132391
23	H	3.889147	4.977037	3.406217	2.118094	1.084089
24	C	5.030002	5.989462	5.221330	4.338514	2.965712
25	H	5.494930	6.458736	5.617817	4.675611	3.351347
26	H	5.070596	6.098449	5.006537	3.934941	2.631840
27	H	5.856781	6.757955	6.152580	5.323895	3.961620

		16	17	18	19	20
16	H	0.000000				
17	H	4.745074	0.000000			
18	H	2.433384	2.474601	0.000000		
19	H	5.572931	4.290217	4.977153	0.000000	
20	H	5.911971	2.500918	4.303981	2.431805	0.000000
21	H	4.744491	9.192930	7.131194	8.089832	9.558486
22	H	5.911616	9.558605	7.973336	7.299907	9.258321
23	H	5.573117	8.090555	7.048287	5.117664	7.300563
24	C	5.447238	6.274790	5.988088	2.607187	4.957038
25	H	5.955436	6.624767	6.446976	2.847883	5.182790
26	H	5.935566	7.222443	6.763167	3.607245	5.956079
27	H	5.932921	6.005265	6.098982	2.017705	4.391046

		21	22	23	24	25
21	H	0.000000				
22	H	2.500962	0.000000			
23	H	4.289970	2.431302	0.000000		
24	C	6.277826	4.961008	2.611989	0.000000	
25	H	6.646905	5.211289	2.876934	1.099483	0.000000

This journal is © The Royal Society of Chemistry 2014

```
   26  H    6.001526   4.383602   2.007093   1.092336   1.766281
   27  H    7.216537   5.950774   3.604303   1.092565   1.766323
                 26         27
   26  H    0.000000
   27  H    1.749346   0.000000
 Stoichiometry    C15H12
 Framework group  C1[X(C15H12)]
 Deg. of freedom    75
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.660011   -0.994497    0.021876
      2          6           0       -2.461890   -1.658725   -0.011206
      3          6           0       -1.218974   -0.948647   -0.021153
      4          6           0       -1.225465    0.498907   -0.012051
      5          6           0       -2.505998    1.146261    0.030743
      6          6           0       -3.677095    0.429690    0.048646
      7          6           0        0.000466   -1.632248   -0.034812
      8          6           0       -0.000122    1.211942   -0.033389
      9          6           0        1.225690    0.499688   -0.012014
     10          6           0        1.219540   -0.948049   -0.021201
     11          6           0        2.462590   -1.657962   -0.011344
     12          1           0        2.433170   -2.745378   -0.025750
     13          6           0        3.660627   -0.993683    0.021768
     14          6           0        3.677475    0.430508    0.048695
     15          6           0        2.506349    1.146963    0.030890
     16          1           0        0.000761   -2.720694   -0.046363
     17          1           0       -4.596123   -1.546706    0.032022
     18          1           0       -2.432401   -2.746140   -0.025547
     19          1           0       -2.558495    2.228612    0.063883
     20          1           0       -4.629014    0.953413    0.086037
     21          1           0        4.596807   -1.545776    0.031838
     22          1           0        4.629307    0.954385    0.086171
     23          1           0        2.559169    2.229250    0.064273
     24          6           0       -0.002164    2.726533   -0.057242
     25          1           0       -0.016095    3.149495    0.957535
     26          1           0        0.877997    3.126685   -0.565563
     27          1           0       -0.871203    3.122773   -0.587772
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3930615      0.4479087
0.3397521
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
```

```
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8799201639 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860565339     A.U. after    8 cycles
            Convg  =    0.8447D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
```

This journal is © The Royal Society of Chemistry 2014

Number	Number	X	Y	Z
1	6	0.000018591	0.000003162	-0.000001985
2	6	-0.000029314	0.000026450	0.000002079
3	6	-0.000043424	0.000007961	0.000006513
4	6	0.000019418	-0.000023202	0.000005675
5	6	0.000030429	-0.000003744	-0.000003017
6	6	0.000016181	-0.000006686	0.000001191
7	6	0.000002601	0.000008318	-0.000008832
8	6	-0.000012962	0.000067819	-0.000011818
9	6	-0.000014225	-0.000021156	-0.000005785
10	6	0.000009859	0.000026204	0.000005901
11	6	-0.000003675	0.000041910	0.000002729
12	1	-0.000002443	-0.000023978	0.000000443
13	6	-0.000009702	-0.000021266	-0.000002901
14	6	-0.000008791	-0.000014658	0.000001110
15	6	0.000003191	-0.000032580	-0.000003211
16	1	0.000008986	-0.000014356	0.000007824
17	1	-0.000011685	-0.000007455	0.000001266
18	1	0.000021175	-0.000010005	0.000001166
19	1	-0.000015597	0.000008546	-0.000001324
20	1	-0.000016141	0.000003022	-0.000002738
21	1	0.000012145	0.000006182	0.000001842
22	1	0.000004615	0.000015725	-0.000003134
23	1	0.000008024	0.000017608	-0.000000621
24	6	0.000078153	-0.000116308	-0.000001598
25	1	-0.000019163	0.000020415	-0.000027187
26	1	-0.000043905	0.000010909	0.000027203
27	1	-0.000002341	0.000031164	0.000009207

Cartesian Forces: Max 0.000116308 RMS 0.000023441

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal Forces: Max 0.000052949 RMS 0.000012888
Search for a local minimum.
Step number 9 out of a maximum of 157
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swaping is turned off.
Update second derivatives using D2CorX and points 1 2 3 4
5
6 7 8 9
DE= -5.21D-08 DEPred=-5.16D-08 R= 1.01D+00
Trust test= 1.01D+00 RLast= 1.20D-02 DXMaxT set to 5.05D-01
Eigenvalues --- 0.00014 0.01481 0.01744 0.01769
0.01795
Eigenvalues --- 0.01819 0.01829 0.01943 0.01976
0.01977

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02019   0.02048   0.02058   0.02110
0.02112
     Eigenvalues ---    0.02143   0.02146   0.02190   0.02226
0.02251
     Eigenvalues ---    0.02347   0.02441   0.06808   0.06895
0.13783
     Eigenvalues ---    0.15773   0.15943   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16004   0.16021   0.16193
0.16221
     Eigenvalues ---    0.20028   0.21970   0.22012   0.22520
0.22609
     Eigenvalues ---    0.23517   0.24455   0.24763   0.24997
0.25941
     Eigenvalues ---    0.28214   0.31987   0.33586   0.33631
0.33658
     Eigenvalues ---    0.33682   0.33682   0.33703   0.33963
0.34027
     Eigenvalues ---    0.35066   0.36967   0.37249   0.37526
0.38086
     Eigenvalues ---    0.38284   0.39451   0.39761   0.40347
0.40910
     Eigenvalues ---    0.41243   0.44490   0.45385   0.47581
0.49643
     Eigenvalues ---    0.49834   0.49892   0.51309   0.54454
0.74292
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     9    8    7    6
5
 RFO step:  Lambda=-3.63022763D-08.
 DIIS coeffs:     -4.29013     14.49440     -7.87863     -1.28249
-0.04314
 Iteration  1 RMS(Cart)=  0.00215045 RMS(Int)=  0.00000763
 Iteration  2 RMS(Cart)=  0.00000791 RMS(Int)=  0.00000008
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000008
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.58954  -0.00001  -0.00011   0.00007  -0.00004
2.58950
    R2        2.69199   0.00000   0.00001  -0.00001   0.00000
2.69199
    R3        2.05394   0.00001   0.00004  -0.00003   0.00001
2.05394
    R4        2.70512  -0.00001   0.00006  -0.00005   0.00001
2.70512
    R5        2.05585   0.00002   0.00005  -0.00002   0.00002
2.05587
    R6        2.73556  -0.00003   0.00006   0.00001   0.00008
2.73564
    R7        2.64192   0.00001  -0.00003   0.00002   0.00000
2.64192
    R8        2.71270  -0.00001   0.00014  -0.00012   0.00002
2.71273
    R9        2.67937   0.00000   0.00010  -0.00010   0.00000
2.67937
   R10        2.59469   0.00000  -0.00005   0.00003  -0.00001
2.59467
   R11        2.04871   0.00002  -0.00003   0.00003   0.00000
2.04870
   R12        2.05436   0.00002   0.00004  -0.00002   0.00002
2.05438
   R13        2.64187   0.00000   0.00002   0.00001   0.00002
2.64190
   R14        2.05698   0.00002   0.00004  -0.00002   0.00002
2.05700
   R15        2.67940   0.00000   0.00008  -0.00010  -0.00002
2.67939
   R16        2.86252  -0.00005  -0.00004  -0.00015  -0.00019
2.86233
   R17        2.73591  -0.00001  -0.00023   0.00010  -0.00013
2.73577
   R18        2.71286   0.00000   0.00001  -0.00008  -0.00007
2.71278
   R19        2.70518  -0.00001   0.00000  -0.00003  -0.00003
2.70515
```

This journal is © The Royal Society of Chemistry 2014

R20	2.05585	0.00002	0.00005	-0.00002	0.00002
2.05587					
R21	2.58945	-0.00002	-0.00003	0.00005	0.00002
2.58947					
R22	2.69200	0.00000	0.00000	-0.00001	-0.00001
2.69199					
R23	2.05393	0.00001	0.00004	-0.00003	0.00001
2.05394					
R24	2.59462	0.00000	0.00001	0.00001	0.00003
2.59464					
R25	2.05436	0.00002	0.00004	-0.00002	0.00002
2.05438					
R26	2.04863	0.00001	0.00003	0.00001	0.00004
2.04867					
R27	2.07772	-0.00001	-0.00005	0.00007	0.00002
2.07774					
R28	2.06422	-0.00003	0.00009	0.00004	0.00013
2.06434					
R29	2.06465	-0.00001	-0.00029	0.00016	-0.00013
2.06452					
A1	2.08926	-0.00001	-0.00008	0.00000	-0.00007
2.08918					
A2	2.10249	0.00001	0.00013	-0.00007	0.00006
2.10255					
A3	2.09143	0.00000	-0.00005	0.00006	0.00002
2.09145					
A4	2.11634	0.00000	0.00004	0.00000	0.00004
2.11638					
A5	2.10426	0.00001	0.00011	-0.00007	0.00005
2.10431					
A6	2.06257	-0.00002	-0.00015	0.00006	-0.00009
2.06248					
A7	2.08529	0.00001	0.00012	-0.00006	0.00006
2.08535					
A8	2.11165	0.00000	-0.00026	0.00013	-0.00013
2.11152					
A9	2.08625	-0.00001	0.00014	-0.00007	0.00007
2.08632					
A10	2.04332	-0.00001	-0.00023	0.00009	-0.00014
2.04318					
A11	2.09314	0.00002	-0.00017	0.00008	-0.00009
2.09304					
A12	2.14669	-0.00001	0.00040	-0.00017	0.00023
2.14692					
A13	2.12455	0.00000	0.00010	-0.00003	0.00007
2.12462					
A14	2.08786	0.00001	0.00015	-0.00002	0.00012
2.08798					
A15	2.07068	-0.00001	-0.00024	0.00005	-0.00019
2.07049					
A16	2.10747	0.00000	0.00006	-0.00002	0.00004
2.10751					

This journal is © The Royal Society of Chemistry 2014

A17	2.08608	0.00000	-0.00003	0.00006	0.00002
2.08610					
A18	2.08964	0.00000	-0.00003	-0.00004	-0.00007
2.08957					
A19	2.11905	0.00000	0.00000	-0.00001	0.00000
2.11905					
A20	2.08206	0.00000	-0.00002	0.00001	-0.00001
2.08205					
A21	2.08202	0.00000	0.00002	0.00000	0.00001
2.08204					
A22	2.08783	-0.00001	-0.00003	0.00000	-0.00003
2.08780					
A23	2.09659	-0.00003	0.00091	-0.00028	0.00063
2.09723					
A24	2.09865	0.00004	-0.00088	0.00028	-0.00061
2.09804					
A25	2.09273	0.00000	0.00018	-0.00003	0.00015
2.09288					
A26	2.14742	0.00002	-0.00024	0.00003	-0.00021
2.14721					
A27	2.04300	-0.00002	0.00005	0.00000	0.00006
2.04305					
A28	2.08651	0.00000	-0.00009	0.00000	-0.00009
2.08642					
A29	2.11129	-0.00001	0.00006	0.00003	0.00008
2.11137					
A30	2.08538	0.00001	0.00004	-0.00003	0.00001
2.08538					
A31	2.06249	-0.00002	-0.00008	0.00004	-0.00004
2.06245					
A32	2.11642	0.00001	-0.00003	0.00002	-0.00001
2.11641					
A33	2.10426	0.00001	0.00011	-0.00007	0.00005
2.10431					
A34	2.08915	-0.00001	0.00001	-0.00002	-0.00001
2.08914					
A35	2.10255	0.00001	0.00008	-0.00005	0.00002
2.10257					
A36	2.09147	0.00000	-0.00009	0.00008	-0.00001
2.09146					
A37	2.10755	0.00000	-0.00001	0.00001	-0.00001
2.10755					
A38	2.08608	0.00000	-0.00003	0.00006	0.00002
2.08610					
A39	2.08955	-0.00001	0.00005	-0.00006	-0.00002
2.08954					
A40	2.12472	0.00001	-0.00005	0.00002	-0.00003
2.12468					
A41	2.08807	0.00001	-0.00004	0.00003	-0.00001
2.08807					
A42	2.07030	-0.00002	0.00010	-0.00006	0.00004
2.07034					

This journal is © The Royal Society of Chemistry 2014

A43	1.94994	0.00003	-0.00007	0.00014	0.00007	1.95002
A44	1.95252	0.00005	-0.00028	0.00008	-0.00020	1.95233
A45	1.95125	0.00003	0.00083	-0.00026	0.00057	1.95182
A46	1.87422	-0.00004	-0.00030	0.00007	-0.00024	1.87398
A47	1.87400	-0.00004	-0.00011	0.00001	-0.00011	1.87389
A48	1.85677	-0.00004	-0.00011	-0.00003	-0.00014	1.85663
D1	-0.00134	0.00000	-0.00003	-0.00001	-0.00003	-0.00137
D2	3.13478	0.00000	0.00004	-0.00004	-0.00001	3.13477
D3	-3.13844	0.00000	-0.00006	0.00005	-0.00002	-3.13846
D4	-0.00232	0.00000	0.00000	0.00001	0.00001	-0.00231
D5	0.00928	0.00000	-0.00017	0.00016	-0.00001	0.00927
D6	-3.12978	0.00000	-0.00020	0.00016	-0.00004	-3.12982
D7	-3.13678	0.00000	-0.00013	0.00010	-0.00003	-3.13680
D8	0.00735	0.00000	-0.00016	0.00011	-0.00006	0.00730
D9	-0.01287	0.00000	0.00019	-0.00015	0.00004	-0.01283
D10	3.12479	0.00000	0.00017	-0.00013	0.00005	3.12484
D11	3.13407	0.00000	0.00012	-0.00011	0.00001	3.13408
D12	-0.01145	0.00000	0.00011	-0.00009	0.00002	-0.01144
D13	0.01873	0.00000	-0.00016	0.00015	0.00000	0.01873
D14	-3.13214	0.00000	-0.00012	0.00012	0.00000	-3.13214
D15	-3.11899	0.00000	-0.00014	0.00013	-0.00001	-3.11900
D16	0.01332	0.00000	-0.00011	0.00010	-0.00001	0.01331
D17	-3.12198	0.00000	-0.00030	0.00021	-0.00009	-3.12207
D18	0.00892	0.00000	-0.00037	0.00022	-0.00015	0.00878
D19	0.01569	0.00000	-0.00032	0.00023	-0.00008	0.01560
D20	-3.13660	0.00000	-0.00038	0.00025	-0.00014	-3.13674

This journal is © The Royal Society of Chemistry 2014

D21	-0.01128	0.00000	-0.00004	-0.00001	-0.00005	-0.01133
D22	3.11519	0.00000	0.00017	-0.00019	-0.00002	3.11517
D23	3.13990	0.00000	-0.00007	0.00002	-0.00005	3.13986
D24	-0.01681	0.00000	0.00014	-0.00016	-0.00002	-0.01683
D25	-0.04183	0.00000	0.00059	-0.00045	0.00014	-0.04169
D26	3.11620	0.00001	0.00094	-0.00055	0.00039	3.11659
D27	3.08991	0.00000	0.00062	-0.00048	0.00014	3.09005
D28	-0.03525	0.00001	0.00097	-0.00058	0.00039	-0.03486
D29	-0.00264	0.00000	0.00020	-0.00015	0.00006	-0.00258
D30	3.13642	0.00000	0.00023	-0.00015	0.00008	3.13650
D31	-3.12926	0.00000	-0.00001	0.00004	0.00003	-3.12923
D32	0.00980	0.00000	0.00002	0.00003	0.00006	0.00985
D33	-0.01562	0.00000	0.00026	-0.00021	0.00004	-0.01558
D34	3.12201	0.00000	0.00027	-0.00020	0.00007	3.12208
D35	3.13666	0.00000	0.00033	-0.00023	0.00010	3.13676
D36	-0.00889	0.00000	0.00034	-0.00021	0.00013	-0.00876
D37	0.04188	0.00000	-0.00064	0.00047	-0.00017	0.04171
D38	-3.08985	0.00000	-0.00068	0.00050	-0.00018	-3.09003
D39	-3.11616	-0.00001	-0.00098	0.00056	-0.00041	-3.11657
D40	0.03529	-0.00001	-0.00101	0.00060	-0.00042	0.03487
D41	1.54945	-0.00001	0.01134	-0.00362	0.00772	1.55717
D42	-2.63181	-0.00001	0.01071	-0.00338	0.00733	-2.62448
D43	-0.55131	0.00000	0.01095	-0.00355	0.00741	-0.54390
D44	-1.57561	-0.00001	0.01169	-0.00372	0.00797	-1.56764
D45	0.52632	0.00000	0.01106	-0.00348	0.00758	0.53390
D46	2.60682	0.00000	0.01130	-0.00364	0.00766	2.61448

```
   D47       -0.01345   0.00000   0.00023  -0.00014   0.00009  -
0.01336
   D48        3.13205   0.00000   0.00021  -0.00016   0.00006
3.13210
   D49        3.11886   0.00000   0.00026  -0.00017   0.00009
3.11895
   D50       -0.01882   0.00000   0.00025  -0.00019   0.00006  -
0.01877
   D51       -3.13981   0.00000  -0.00001   0.00000  -0.00001  -
3.13982
   D52        0.01698   0.00000  -0.00029   0.00021  -0.00009
0.01689
   D53        0.01138   0.00000  -0.00005   0.00004  -0.00001
0.01137
   D54       -3.11502   0.00000  -0.00033   0.00024  -0.00009  -
3.11511
   D55        0.01149   0.00000  -0.00015   0.00010  -0.00005
0.01144
   D56       -3.12472   0.00000  -0.00024   0.00015  -0.00009  -
3.12482
   D57       -3.13407   0.00000  -0.00013   0.00012  -0.00002  -
3.13408
   D58        0.01291   0.00000  -0.00023   0.00017  -0.00006
0.01285
   D59        0.00136   0.00000   0.00001   0.00001   0.00002
0.00138
   D60        3.13844   0.00000   0.00007  -0.00005   0.00002
3.13846
   D61       -3.13472   0.00000  -0.00009   0.00006  -0.00003  -
3.13475
   D62        0.00236   0.00000  -0.00003   0.00000  -0.00003
0.00233
   D63       -0.00930   0.00000   0.00020  -0.00017   0.00003  -
0.00928
   D64        3.12971   0.00000   0.00025  -0.00017   0.00008
3.12979
   D65        3.13677   0.00000   0.00013  -0.00011   0.00003
3.13680
   D66       -0.00740   0.00000   0.00019  -0.00011   0.00008  -
0.00731
   D67        0.00259   0.00000  -0.00017   0.00014  -0.00003
0.00256
   D68        3.12914   0.00000   0.00010  -0.00006   0.00005
3.12919
   D69       -3.13642   0.00000  -0.00023   0.00014  -0.00008  -
3.13650
   D70       -0.00987   0.00000   0.00005  -0.00006  -0.00001  -
0.00988
         Item               Value     Threshold  Converged?
 Maximum Force            0.000053     0.000450     YES
 RMS     Force            0.000013     0.000300     YES
 Maximum Displacement     0.014893     0.001800     NO
```

RMS Displacement 0.002150 0.001200 NO
Predicted change in Energy=-3.051829D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.791995	-5.432745	0.005383
2	6	0	-3.422410	-5.398348	-0.022700
3	6	0	-2.710612	-4.156421	-0.033631
4	6	0	-3.449643	-2.911639	-0.030873
5	6	0	-4.881788	-3.002371	0.006904
6	6	0	-5.528395	-4.213479	0.025886
7	6	0	-1.312883	-4.128102	-0.042225
8	6	0	-2.754266	-1.676209	-0.053238
9	6	0	-1.336659	-1.669344	-0.026822
10	6	0	-0.608458	-2.920575	-0.029633
11	6	0	0.822856	-2.902785	-0.014645
12	1	0	1.348455	-3.855267	-0.024288
13	6	0	1.519051	-1.722967	0.017391
14	6	0	0.811883	-0.486518	0.038008
15	6	0	-0.560741	-0.462294	0.015210
16	1	0	-0.761212	-5.066442	-0.048880
17	1	0	-5.319300	-6.383104	0.016330
18	1	0	-2.845871	-6.320890	-0.032223
19	1	0	-5.475760	-2.095880	0.035246
20	1	0	-6.614581	-4.244129	0.059285
21	1	0	2.605860	-1.724556	0.031388
22	1	0	1.366902	0.447544	0.074570
23	1	0	-1.063744	0.497637	0.043815
24	6	0	-3.522287	-0.371029	-0.083216
25	1	0	-3.744978	-0.006439	0.929882
26	1	0	-2.966821	0.416033	-0.598324
27	1	0	-4.474034	-0.471694	-0.610086

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370304	0.000000			
3	C	2.441860	1.431489	0.000000		
4	C	2.856431	2.486872	1.447638	0.000000	
5	C	2.432033	2.805595	2.459162	1.435513	0.000000
6	C	1.424540	2.416908	2.818989	2.453409	1.373042
7	C	3.715990	2.462522	1.398042	2.458791	3.742561
8	C	4.274030	3.781754	2.480673	1.417863	2.507722
9	C	5.109165	4.272686	2.841363	2.451125	3.787616
10	C	4.879980	3.749365	2.438520	2.841200	4.274269
11	C	6.158543	4.924448	3.749314	4.272539	5.705553

This journal is © The Royal Society of Chemistry 2014

12	H	6.339909	5.014206	4.070234	4.890013	6.288429
13	C	7.320648	6.158577	4.879994	5.109128	6.527459
14	C	7.474602	6.485291	5.087366	4.903730	6.224819
15	C	6.527556	5.705718	4.274448	3.787766	5.012336
16	H	4.047757	2.681944	2.151402	3.445456	4.608975
17	H	1.086901	2.137629	3.430141	3.943211	3.408939
18	H	2.139536	1.087921	2.168692	3.462302	3.893463
19	H	3.406331	3.889203	3.449147	2.185173	1.084127
20	H	2.176588	3.395423	3.906060	3.435184	2.132435
21	H	8.275240	7.059725	5.846628	6.171075	7.595938
22	H	8.515551	7.557872	6.150961	5.873189	7.138110
23	H	7.005052	6.350620	4.937451	4.161881	5.179660
24	C	5.219288	5.028675	3.871752	2.542187	2.963161
25	H	5.603190	5.484901	4.384132	3.074160	3.334641
26	H	6.156617	5.860541	4.614310	3.410062	3.964705
27	H	5.009184	5.071770	4.125429	2.708910	2.636525

		6	7	8	9	10
6	C	0.000000				
7	C	4.216927	0.000000			
8	C	3.760291	2.844201	0.000000		
9	C	4.903677	2.458920	1.417870	0.000000	
10	C	5.087285	1.398032	2.480624	1.447710	0.000000
11	C	6.485210	2.462426	3.781769	2.486971	1.431502
12	H	6.886356	2.675347	4.645584	3.462384	2.168683
13	C	7.474571	3.715922	4.274156	2.856555	2.441878
14	C	7.354557	4.216895	3.760467	2.453470	2.818968
15	C	6.224877	3.742614	2.507953	1.435544	2.459153
16	H	4.843467	1.088517	3.932679	3.445562	2.151383
17	H	2.179698	4.597809	5.360886	6.171128	5.846645
18	H	3.411817	2.675532	4.645631	4.890258	4.070401
19	H	2.118274	4.633084	2.755083	4.161483	4.937100
20	H	1.087132	5.303939	4.637769	5.873108	6.150871
21	H	8.506519	4.597716	5.361012	3.943335	3.430164
22	H	8.323018	5.303907	4.637962	3.435221	3.906038
23	H	6.490612	4.633242	2.755520	2.185241	3.449181
24	C	4.335988	4.358754	1.514678	2.542789	3.872139
25	H	4.658001	4.883460	2.176274	3.079048	4.387553
26	H	5.327634	4.867640	2.172505	2.707923	4.125317
27	H	3.939174	4.866688	2.172220	3.408472	4.612659

		11	12	13	14	15
11	C	0.000000				
12	H	1.087920	0.000000			
13	C	1.370286	2.139520	0.000000		
14	C	2.416866	3.411783	1.424542	0.000000	
15	C	2.805571	3.893438	2.432043	1.373027	0.000000
16	H	2.681764	2.432744	4.047569	4.843334	4.608956
17	H	7.059721	7.130959	8.275260	8.506563	7.596044
18	H	5.014310	4.865360	6.340023	6.886508	6.288658
19	H	6.350287	7.047617	7.004767	6.490339	5.179422
20	H	7.557786	7.972964	8.515514	8.323008	7.138151
21	H	2.137626	2.474692	1.086900	2.179710	3.408948
22	H	3.395387	4.303987	2.176589	1.087131	2.132402

23	H	3.889157	4.977059	3.406260	2.118152	1.084111
24	C	5.029389	5.988950	5.220435	4.337403	2.964587
25	H	5.490542	6.454997	5.611516	4.668072	3.344218
26	H	5.071182	6.098782	5.007742	3.936765	2.633839
27	H	5.858480	6.759668	6.154386	5.325520	3.962947

		16	17	18	19	20
16	H	0.000000				
17	H	4.744894	0.000000			
18	H	2.433047	2.474688	0.000000		
19	H	5.572996	4.290120	4.977105	0.000000	
20	H	5.911838	2.500962	4.304008	2.431556	0.000000
21	H	4.744662	9.192957	7.131038	8.090146	9.558533
22	H	5.911697	9.558580	7.973115	7.300176	9.258299
23	H	5.573069	8.090433	7.047983	5.117840	7.300437
24	C	5.447166	6.275684	5.988404	2.608677	4.958174
25	H	5.955205	6.631359	6.450296	2.856876	5.191394
26	H	5.934993	7.220819	6.761748	3.606368	5.954470
27	H	5.933946	6.004302	6.099011	2.014420	4.388766

		21	22	23	24	25
21	H	0.000000				
22	H	2.500979	0.000000			
23	H	4.290021	2.431357	0.000000		
24	C	6.276890	4.959751	2.610585	0.000000	
25	H	6.640207	5.202786	2.868488	1.099493	0.000000
26	H	6.002785	4.385765	2.010150	1.092404	1.766190
27	H	7.218451	5.952334	3.605172	1.092496	1.766207

		26	27
26	H	0.000000	
27	H	1.749254	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.660202	-0.994282	0.021755
2	6	0	-2.462085	-1.658485	-0.011163
3	6	0	-1.219147	-0.948437	-0.021080
4	6	0	-1.225518	0.499160	-0.012072
5	6	0	-2.506098	1.146454	0.030604
6	6	0	-3.677203	0.429907	0.048425
7	6	0	0.000185	-1.632225	-0.034628
8	6	0	-0.000049	1.211976	-0.033382
9	6	0	1.225608	0.499470	-0.012054
10	6	0	1.219373	-0.948198	-0.021095
11	6	0	2.462363	-1.658182	-0.011214
12	1	0	2.432833	-2.745608	-0.025495

```
     13          6           0        3.660447   -0.993958    0.021714
     14          6           0        3.677354    0.430233    0.048442
     15          6           0        2.506237    1.146732    0.030659
     16          1           0        0.000302   -2.720682   -0.045975
     17          1           0       -4.596342   -1.546452    0.031864
     18          1           0       -2.432527   -2.745911   -0.025422
     19          1           0       -2.558786    2.228794    0.063698
     20          1           0       -4.629092    0.953718    0.085648
     21          1           0        4.596615   -1.546081    0.031790
     22          1           0        4.629208    0.954105    0.085695
     23          1           0        2.559054    2.229048    0.063843
     24          6           0       -0.000860    2.726473   -0.056831
     25          1           0       -0.006433    3.149261    0.958109
     26          1           0        0.875983    3.125767   -0.571668
     27          1           0       -0.873247    3.124217   -0.580557
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3930859      0.4479112
0.3397539
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8835852872 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860565216     A.U. after    8 cycles
            Convg  =    0.9562D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6           0.000015873    0.000003134   -0.000000127
      2          6          -0.000020461    0.000013628    0.000001177
      3          6          -0.000022425    0.000006214    0.000002256
      4          6           0.000011666   -0.000015727    0.000002008
      5          6           0.000008837   -0.000005813   -0.000001571
      6          6           0.000008822   -0.000000717   -0.000000411
      7          6           0.000000373    0.000004610   -0.000002985
      8          6          -0.000005726    0.000028212   -0.000000336
      9          6          -0.000002603   -0.000014937   -0.000003007
     10          6           0.000004057    0.000015827    0.000001803
     11          6           0.000000164    0.000026120    0.000001685
     12          1          -0.000000729   -0.000014492    0.000000796
     13          6          -0.000009751   -0.000015301   -0.000000591
     14          6          -0.000006010   -0.000006884   -0.000000496
     15          6           0.000006947   -0.000011891   -0.000001578
     16          1           0.000005371   -0.000008750    0.000004143
     17          1          -0.000007808   -0.000005161    0.000000707
     18          1           0.000012671   -0.000006688    0.000001189
     19          1          -0.000007301    0.000004044   -0.000001713
     20          1          -0.000009718    0.000000083   -0.000001154
     21          1           0.000008274    0.000004146    0.000001040
     22          1           0.000004367    0.000008615   -0.000001306
     23          1           0.000003587    0.000008234   -0.000001203
     24          6           0.000030376   -0.000045297   -0.000004049
     25          1          -0.000008486    0.000009440   -0.000020770
     26          1          -0.000023961    0.000002646    0.000015861
     27          1           0.000003594    0.000016706    0.000008631
```

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000045297 RMS     0.000011384


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000025330 RMS     0.000006785
 Search for a local minimum.
 Step number  10 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8    9
10
 DE=  1.24D-07 DEPred=-3.05D-07 R=-4.05D-01
 Trust test=-4.05D-01 RLast= 1.87D-02 DXMaxT set to 2.52D-01
     Eigenvalues ---   -0.01509   0.00000   0.01501   0.01769
0.01775
     Eigenvalues ---    0.01801   0.01819   0.01829   0.01958
0.01976
     Eigenvalues ---    0.01979   0.02022   0.02052   0.02106
0.02111
     Eigenvalues ---    0.02143   0.02146   0.02188   0.02226
0.02254
     Eigenvalues ---    0.02346   0.02430   0.04584   0.06827
0.07331
     Eigenvalues ---    0.14111   0.15835   0.15996   0.15999
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16008   0.16049
0.16194
     Eigenvalues ---    0.16249   0.21694   0.21998   0.22464
0.22608
     Eigenvalues ---    0.23498   0.23838   0.24459   0.24993
0.25103
     Eigenvalues ---    0.28172   0.31463   0.32660   0.33586
0.33631
     Eigenvalues ---    0.33655   0.33682   0.33682   0.33733
0.33963
     Eigenvalues ---    0.34022   0.35577   0.36968   0.37255
0.37616
     Eigenvalues ---    0.38078   0.38329   0.39477   0.39924
0.40510
     Eigenvalues ---    0.41108   0.41238   0.44488   0.45385
0.49504
     Eigenvalues ---    0.49699   0.49785   0.49834   0.51310
0.56023
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is  -1.51D-02 should be greater than     0.000000
Eigenvector:
                          D40       D28       D26       D39       A44
   1                    0.28219  -0.27866  -0.27752   0.27579  -
0.23881
                          A47       A46       D42       A45       R16
   1                    0.23350   0.22979   0.20714  -0.19632
0.17322
 Eigenvalue     2 is   1.83D-07 Eigenvector:
                          D44       D46       D45       D41       D43
   1                    0.42417   0.41801   0.39468   0.39030
0.38414
                          D42       D40       D28       D39       D26
   1                    0.36082  -0.08315   0.08252  -0.07997
0.07888
 Use linear search instead of GDIIS.
 RFO step:  Lambda=-3.31917604D-07 EMin= 1.50948329D-02
 Skip linear search -- no minimum in search direction.
 Iteration  1 RMS(Cart)=  0.00439175 RMS(Int)=  0.00002297
 Iteration  2 RMS(Cart)=  0.00002384 RMS(Int)=  0.00000047
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000047
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
```

This journal is © The Royal Society of Chemistry 2014

R1	2.58950	-0.00001	0.00000	-0.00027	-0.00027
2.58923					
R2	2.69199	0.00000	0.00000	-0.00012	-0.00012
2.69187					
R3	2.05394	0.00001	0.00000	0.00026	0.00026
2.05421					
R4	2.70512	0.00000	0.00000	-0.00013	-0.00013
2.70500					
R5	2.05587	0.00001	0.00000	0.00040	0.00040
2.05627					
R6	2.73564	-0.00002	0.00000	-0.00030	-0.00030
2.73534					
R7	2.64192	0.00000	0.00000	0.00010	0.00010
2.64202					
R8	2.71273	0.00000	0.00000	-0.00001	-0.00001
2.71272					
R9	2.67937	0.00001	0.00000	0.00032	0.00032
2.67969					
R10	2.59467	0.00000	0.00000	0.00009	0.00009
2.59477					
R11	2.04870	0.00001	0.00000	0.00018	0.00018
2.04889					
R12	2.05438	0.00001	0.00000	0.00032	0.00032
2.05470					
R13	2.64190	0.00000	0.00000	0.00012	0.00012
2.64202					
R14	2.05700	0.00001	0.00000	0.00033	0.00033
2.05733					
R15	2.67939	0.00001	0.00000	0.00024	0.00024
2.67962					
R16	2.86233	-0.00001	0.00000	-0.00167	-0.00167
2.86066					
R17	2.73577	-0.00001	0.00000	-0.00056	-0.00056
2.73521					
R18	2.71278	0.00001	0.00000	-0.00012	-0.00012
2.71266					
R19	2.70515	0.00000	0.00000	-0.00018	-0.00018
2.70497					
R20	2.05587	0.00001	0.00000	0.00040	0.00040
2.05628					
R21	2.58947	-0.00001	0.00000	-0.00020	-0.00020
2.58927					
R22	2.69199	0.00000	0.00000	-0.00012	-0.00012
2.69187					
R23	2.05394	0.00001	0.00000	0.00026	0.00026
2.05421					
R24	2.59464	0.00000	0.00000	0.00015	0.00015
2.59479					
R25	2.05438	0.00001	0.00000	0.00032	0.00032
2.05470					
R26	2.04867	0.00001	0.00000	0.00026	0.00026
2.04893					

This journal is © The Royal Society of Chemistry 2014

R27	2.07774	-0.00001	0.00000	-0.00018	-0.00018
2.07756					
R28	2.06434	-0.00002	0.00000	-0.00017	-0.00017
2.06417					
R29	2.06452	-0.00001	0.00000	-0.00054	-0.00054
2.06398					
A1	2.08918	0.00000	0.00000	-0.00045	-0.00045
2.08874					
A2	2.10255	0.00001	0.00000	0.00050	0.00050
2.10305					
A3	2.09145	0.00000	0.00000	-0.00005	-0.00005
2.09139					
A4	2.11638	0.00000	0.00000	0.00018	0.00018
2.11656					
A5	2.10431	0.00001	0.00000	0.00061	0.00061
2.10492					
A6	2.06248	-0.00001	0.00000	-0.00079	-0.00079
2.06169					
A7	2.08535	0.00001	0.00000	0.00046	0.00046
2.08580					
A8	2.11152	0.00000	0.00000	-0.00053	-0.00053
2.11099					
A9	2.08632	0.00000	0.00000	0.00007	0.00007
2.08639					
A10	2.04318	-0.00001	0.00000	-0.00063	-0.00063
2.04255					
A11	2.09304	0.00001	0.00000	0.00008	0.00008
2.09312					
A12	2.14692	0.00000	0.00000	0.00055	0.00055
2.14747					
A13	2.12462	0.00000	0.00000	0.00027	0.00027
2.12488					
A14	2.08798	0.00000	0.00000	0.00067	0.00067
2.08865					
A15	2.07049	0.00000	0.00000	-0.00092	-0.00092
2.06957					
A16	2.10751	0.00000	0.00000	0.00018	0.00018
2.10769					
A17	2.08610	0.00000	0.00000	0.00020	0.00020
2.08631					
A18	2.08957	0.00000	0.00000	-0.00038	-0.00038
2.08918					
A19	2.11905	0.00000	0.00000	0.00002	0.00002
2.11907					
A20	2.08205	0.00000	0.00000	-0.00003	-0.00003
2.08202					
A21	2.08204	0.00000	0.00000	0.00000	0.00000
2.08204					
A22	2.08780	-0.00001	0.00000	-0.00036	-0.00036
2.08744					
A23	2.09723	-0.00001	0.00000	0.00103	0.00103
2.09826					

```
   A24        2.09804   0.00002   0.00000  -0.00069  -0.00069
2.09735
   A25        2.09288   0.00000   0.00000   0.00043   0.00043
2.09331
   A26        2.14721   0.00001   0.00000  -0.00007  -0.00007
2.14714
   A27        2.04305  -0.00001   0.00000  -0.00036  -0.00036
2.04269
   A28        2.08642   0.00000   0.00000  -0.00016  -0.00016
2.08626
   A29        2.11137  -0.00001   0.00000  -0.00021  -0.00021
2.11116
   A30        2.08538   0.00001   0.00000   0.00037   0.00037
2.08575
   A31        2.06245  -0.00001   0.00000  -0.00073  -0.00073
2.06172
   A32        2.11641   0.00000   0.00000   0.00012   0.00012
2.11653
   A33        2.10431   0.00001   0.00000   0.00061   0.00061
2.10492
   A34        2.08914  -0.00001   0.00000  -0.00036  -0.00036
2.08878
   A35        2.10257   0.00001   0.00000   0.00044   0.00044
2.10302
   A36        2.09146   0.00000   0.00000  -0.00008  -0.00008
2.09138
   A37        2.10755   0.00000   0.00000   0.00011   0.00011
2.10766
   A38        2.08610   0.00000   0.00000   0.00021   0.00021
2.08631
   A39        2.08954   0.00000   0.00000  -0.00032  -0.00032
2.08922
   A40        2.12468   0.00000   0.00000   0.00013   0.00013
2.12481
   A41        2.08807   0.00001   0.00000   0.00048   0.00048
2.08854
   A42        2.07034  -0.00001   0.00000  -0.00059  -0.00059
2.06975
   A43        1.95002   0.00002   0.00000   0.00109   0.00109
1.95110
   A44        1.95233   0.00003   0.00000   0.00166   0.00166
1.95398
   A45        1.95182   0.00002   0.00000   0.00273   0.00273
1.95455
   A46        1.87398  -0.00002   0.00000  -0.00239  -0.00239
1.87159
   A47        1.87389  -0.00002   0.00000  -0.00219  -0.00219
1.87170
   A48        1.85663  -0.00002   0.00000  -0.00134  -0.00134
1.85529
    D1       -0.00137   0.00000   0.00000  -0.00022  -0.00022  -
0.00160
```

This journal is © The Royal Society of Chemistry 2014

D2	3.13477	0.00000	0.00000	0.00015	0.00015	3.13492
D3	-3.13846	0.00000	0.00000	-0.00037	-0.00037	-3.13883
D4	-0.00231	0.00000	0.00000	0.00000	0.00000	-0.00231
D5	0.00927	0.00000	0.00000	-0.00046	-0.00046	0.00881
D6	-3.12982	0.00000	0.00000	-0.00062	-0.00062	-3.13044
D7	-3.13680	0.00000	0.00000	-0.00031	-0.00031	-3.13711
D8	0.00730	0.00000	0.00000	-0.00047	-0.00047	0.00682
D9	-0.01283	0.00000	0.00000	0.00069	0.00069	-0.01214
D10	3.12484	0.00000	0.00000	0.00081	0.00081	3.12565
D11	3.13408	0.00000	0.00000	0.00033	0.00033	3.13440
D12	-0.01144	0.00000	0.00000	0.00044	0.00044	-0.01099
D13	0.01873	0.00000	0.00000	-0.00050	-0.00050	0.01823
D14	-3.13214	0.00000	0.00000	-0.00040	-0.00040	-3.13254
D15	-3.11900	0.00000	0.00000	-0.00062	-0.00062	-3.11961
D16	0.01331	0.00000	0.00000	-0.00051	-0.00051	0.01280
D17	-3.12207	0.00000	0.00000	-0.00106	-0.00106	-3.12313
D18	0.00878	0.00000	0.00000	-0.00127	-0.00127	0.00751
D19	0.01560	0.00000	0.00000	-0.00094	-0.00094	0.01466
D20	-3.13674	0.00000	0.00000	-0.00115	-0.00115	-3.13788
D21	-0.01133	0.00000	0.00000	-0.00016	-0.00016	-0.01149
D22	3.11517	0.00000	0.00000	0.00059	0.00059	3.11575
D23	3.13986	0.00000	0.00000	-0.00026	-0.00026	3.13960
D24	-0.01683	0.00000	0.00000	0.00048	0.00048	-0.01635
D25	-0.04169	0.00000	0.00000	0.00200	0.00200	-0.03968
D26	3.11659	0.00000	0.00000	0.00333	0.00333	3.11992
D27	3.09005	0.00000	0.00000	0.00211	0.00211	3.09215

This journal is © The Royal Society of Chemistry 2014

D28	-0.03486	0.00000	0.00000	0.00343	0.00343	-0.03143
D29	-0.00258	0.00000	0.00000	0.00065	0.00065	-0.00194
D30	3.13650	0.00000	0.00000	0.00081	0.00081	3.13731
D31	-3.12923	0.00000	0.00000	-0.00010	-0.00010	-3.12933
D32	0.00985	0.00000	0.00000	0.00007	0.00007	0.00992
D33	-0.01558	0.00000	0.00000	0.00089	0.00089	-0.01469
D34	3.12208	0.00000	0.00000	0.00101	0.00101	3.12309
D35	3.13676	0.00000	0.00000	0.00110	0.00110	3.13786
D36	-0.00876	0.00000	0.00000	0.00121	0.00121	-0.00755
D37	0.04171	0.00000	0.00000	-0.00205	-0.00205	0.03966
D38	-3.09003	0.00000	0.00000	-0.00216	-0.00216	-3.09219
D39	-3.11657	0.00000	0.00000	-0.00336	-0.00335	-3.11993
D40	0.03487	0.00000	0.00000	-0.00347	-0.00347	0.03140
D41	1.55717	0.00000	0.00000	0.01245	0.01245	1.56962
D42	-2.62448	0.00000	0.00000	0.01130	0.01130	-2.61318
D43	-0.54390	0.00000	0.00000	0.01259	0.01259	-0.53130
D44	-1.56764	0.00000	0.00000	0.01378	0.01378	-1.55386
D45	0.53390	0.00000	0.00000	0.01263	0.01263	0.54652
D46	2.61448	0.00000	0.00000	0.01392	0.01392	2.62840
D47	-0.01336	0.00000	0.00000	0.00061	0.00061	-0.01275
D48	3.13210	0.00000	0.00000	0.00050	0.00050	3.13261
D49	3.11895	0.00000	0.00000	0.00072	0.00073	3.11968
D50	-0.01877	0.00000	0.00000	0.00061	0.00061	-0.01815
D51	-3.13982	0.00000	0.00000	0.00015	0.00015	-3.13967
D52	0.01689	0.00000	0.00000	-0.00066	-0.00066	0.01623
D53	0.01137	0.00000	0.00000	0.00003	0.00003	0.01139

```
   D54       -3.11511   0.00000   0.00000  -0.00078  -0.00078  -
3.11588
   D55        0.01144   0.00000   0.00000  -0.00040  -0.00040
0.01104
   D56       -3.12482   0.00000   0.00000  -0.00084  -0.00084  -
3.12565
   D57       -3.13408   0.00000   0.00000  -0.00029  -0.00029  -
3.13437
   D58        0.01285   0.00000   0.00000  -0.00072  -0.00072
0.01212
   D59        0.00138   0.00000   0.00000   0.00018   0.00018
0.00156
   D60        3.13846   0.00000   0.00000   0.00032   0.00032
3.13878
   D61       -3.13475   0.00000   0.00000  -0.00027  -0.00027  -
3.13502
   D62        0.00233   0.00000   0.00000  -0.00013  -0.00013
0.00220
   D63       -0.00928   0.00000   0.00000   0.00049   0.00049  -
0.00879
   D64        3.12979   0.00000   0.00000   0.00069   0.00069
3.13049
   D65        3.13680   0.00000   0.00000   0.00035   0.00035
3.13715
   D66       -0.00731   0.00000   0.00000   0.00055   0.00055  -
0.00676
   D67        0.00256   0.00000   0.00000  -0.00059  -0.00059
0.00198
   D68        3.12919   0.00000   0.00000   0.00022   0.00022
3.12941
   D69       -3.13650   0.00000   0.00000  -0.00079  -0.00079  -
3.13729
   D70       -0.00988   0.00000   0.00000   0.00002   0.00002  -
0.00987
         Item               Value     Threshold  Converged?
 Maximum Force            0.000025     0.000450     YES
 RMS     Force            0.000007     0.000300     YES
 Maximum Displacement     0.030977     0.001800     NO
 RMS     Displacement     0.004392     0.001200     NO
 Predicted change in Energy=-3.972303D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.791650   -5.433730    0.003524
      2          6           0       -3.422185   -5.398394   -0.022243
      3          6           0       -2.711046   -4.156162   -0.032800
```

4	6	0	-3.450069	-2.911559	-0.031275
5	6	0	-4.882204	-3.003273	0.004319
6	6	0	-5.528357	-4.214697	0.022216
7	6	0	-1.313256	-4.127862	-0.039998
8	6	0	-2.754745	-1.675891	-0.052797
9	6	0	-1.337004	-1.669408	-0.026782
10	6	0	-0.608777	-2.920283	-0.028296
11	6	0	0.822445	-2.902812	-0.013100
12	1	0	1.347231	-3.855998	-0.021503
13	6	0	1.519008	-1.723285	0.017087
14	6	0	0.811872	-0.486860	0.035740
15	6	0	-0.560837	-0.462533	0.013456
16	1	0	-0.761520	-5.066383	-0.044640
17	1	0	-5.318854	-6.384310	0.013874
18	1	0	-2.844314	-6.320365	-0.030525
19	1	0	-5.477513	-2.097497	0.031157
20	1	0	-6.614781	-4.245391	0.053200
21	1	0	2.605958	-1.724757	0.030980
22	1	0	1.366793	0.447536	0.070190
23	1	0	-1.063219	0.497926	0.040336
24	6	0	-3.521127	-0.370703	-0.079695
25	1	0	-3.731599	-0.000075	0.933719
26	1	0	-2.971961	0.414622	-0.603935
27	1	0	-4.479717	-0.469871	-0.593694

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370163	0.000000			
3	C	2.441805	1.431423	0.000000		
4	C	2.856991	2.487007	1.447478	0.000000	
5	C	2.432143	2.805167	2.458548	1.435510	0.000000
6	C	1.424474	2.416417	2.818456	2.453632	1.373092
7	C	3.715698	2.462144	1.398096	2.458748	3.742200
8	C	4.274752	3.781989	2.480736	1.418032	2.508244
9	C	5.109365	4.272392	2.841121	2.451123	3.787956
10	C	4.880047	3.749178	2.438637	2.841308	4.274358
11	C	6.158237	4.923911	3.749244	4.272562	5.705560
12	H	6.338432	5.012616	4.069378	4.889392	6.287581
13	C	7.320655	6.158194	4.880034	5.109409	6.527944
14	C	7.474759	6.484888	5.087183	4.903856	6.225418
15	C	6.527839	5.705376	4.274159	3.787795	5.012949
16	H	4.047124	2.681394	2.151579	3.445539	4.608563
17	H	1.087039	2.137917	3.430377	3.943906	3.409130
18	H	2.139953	1.088134	2.168304	3.462210	3.893239
19	H	3.406115	3.888849	3.448990	2.185663	1.084225
20	H	2.176792	3.395258	3.905701	3.435352	2.132385
21	H	8.275376	7.059529	5.846908	6.171535	7.596571
22	H	8.515876	7.557628	6.150887	5.873327	7.138795
23	H	7.006218	6.351002	4.937734	4.162544	5.181152
24	C	5.220670	5.028992	3.871451	2.542311	2.964796
25	H	5.613695	5.491033	4.387339	3.080132	3.347667

This journal is © The Royal Society of Chemistry 2014

26	H	6.154956	5.859370	4.613711	3.408813	3.962450
27	H	5.009378	5.072994	4.126929	2.708936	2.633960
		6	7	8	9	10
6	C	0.000000				
7	C	4.216455	0.000000			
8	C	3.760862	2.844331	0.000000		
9	C	4.903910	2.458604	1.417995	0.000000	
10	C	5.087271	1.398096	2.480785	1.447413	0.000000
11	C	6.484980	2.462252	3.781957	2.486904	1.431409
12	H	6.885077	2.674405	4.645434	3.462127	2.168312
13	C	7.474791	3.715772	4.274587	2.856857	2.441788
14	C	7.354961	4.216491	3.760637	2.453568	2.818491
15	C	6.225357	3.742142	2.507959	1.435480	2.458572
16	H	4.842785	1.088694	3.932995	3.445422	2.151590
17	H	2.179721	4.597748	5.361745	6.171474	5.846887
18	H	3.411848	2.674192	4.645392	4.889110	4.069176
19	H	2.117830	4.633410	2.756495	4.162983	4.938128
20	H	1.087299	5.303647	4.638258	5.873416	6.150987
21	H	8.506877	4.597846	5.361581	3.943774	3.430352
22	H	8.323569	5.303684	4.638011	3.435313	3.905737
23	H	6.492041	4.633237	2.755978	2.185589	3.448968
24	C	4.337701	4.358041	1.513797	2.541620	3.871019
25	H	4.671425	4.882124	2.176193	3.072999	4.382363
26	H	5.325206	4.868622	2.172827	2.710972	4.127661
27	H	3.937349	4.869698	2.173150	3.411294	4.616100
		11	12	13	14	15
11	C	0.000000				
12	H	1.088134	0.000000			
13	C	1.370181	2.139968	0.000000		
14	C	2.416469	3.411888	1.424478	0.000000	
15	C	2.805198	3.893271	2.432132	1.373105	0.000000
16	H	2.681600	2.431542	4.047335	4.842938	4.608588
17	H	7.059541	7.129538	8.275356	8.506833	7.596458
18	H	5.012494	4.862329	6.338296	6.884902	6.287321
19	H	6.351374	7.047853	7.006535	6.492344	5.181421
20	H	7.557727	7.971878	8.515917	8.323583	7.138756
21	H	2.137914	2.475750	1.087040	2.179715	3.409121
22	H	3.395303	4.304555	2.176799	1.087299	2.132417
23	H	3.888907	4.977023	3.406202	2.117969	1.084247
24	C	5.028183	5.987619	5.219369	4.336093	2.963179
25	H	5.482851	6.447876	5.601655	4.656872	3.333839
26	H	5.074639	6.101872	5.012495	3.941984	2.638956
27	H	5.862526	6.763623	6.158637	5.328920	3.965641
		16	17	18	19	20
16	H	0.000000				
17	H	4.744434	0.000000			
18	H	2.431194	2.475764	0.000000		
19	H	5.573205	4.289783	4.976963	0.000000	
20	H	5.911367	2.501189	4.304526	2.430497	0.000000
21	H	4.744691	9.193170	7.129437	8.092060	9.559086
22	H	5.911531	9.559036	7.971703	7.302276	9.259015
23	H	5.573130	8.091743	7.047441	5.120771	7.301990

This journal is © The Royal Society of Chemistry 2014

24	C	5.446657	6.277265	5.988237	2.611810	4.959996
25	H	5.953656	6.642586	6.454697	2.874371	5.206799
26	H	5.936351	7.219077	6.760558	3.604424	5.951276
27	H	5.937539	6.004489	6.100819	2.008781	4.385376

		21	22	23	24	25
21	H	0.000000				
22	H	2.501184	0.000000			
23	H	4.289903	2.430718	0.000000		
24	C	6.275897	4.958200	2.609643	0.000000	
25	H	6.629788	5.190341	2.857689	1.099396	0.000000
26	H	6.007764	4.390935	2.016264	1.092313	1.764485
27	H	7.223002	5.955171	3.607088	1.092211	1.764477

		26	27
26	H	0.000000	
27	H	1.748074	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.660469	-0.994498	0.020581
2	6	0	-2.462114	-1.658076	-0.010356
3	6	0	-1.219450	-0.947679	-0.020032
4	6	0	-1.225615	0.499764	-0.012034
5	6	0	-2.506552	1.146465	0.028808
6	6	0	-3.677566	0.429652	0.045662
7	6	0	-0.000211	-1.631763	-0.032530
8	6	0	0.000068	1.212568	-0.032633
9	6	0	1.225508	0.499417	-0.012059
10	6	0	1.219187	-0.947960	-0.020022
11	6	0	2.461797	-1.658423	-0.010287
12	1	0	2.430991	-2.746042	-0.023489
13	6	0	3.660186	-0.994872	0.020654
14	6	0	3.677395	0.429282	0.045634
15	6	0	2.506398	1.146149	0.028707
16	1	0	-0.000345	-2.720415	-0.042032
17	1	0	-4.596744	-1.546722	0.030191
18	1	0	-2.431338	-2.745695	-0.023550
19	1	0	-2.560534	2.228880	0.060578
20	1	0	-4.629575	0.953741	0.080741
21	1	0	4.596426	-1.547155	0.030357
22	1	0	4.629441	0.953305	0.080669
23	1	0	2.560236	2.228597	0.060321
24	6	0	0.000977	2.726231	-0.052775
25	1	0	0.009284	3.147873	0.962518
26	1	0	0.871471	3.127164	-0.576836

```
     27          1           0       -0.876550    3.128931   -0.563366
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3932319      0.4479017
0.3397445
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8956720659 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
```

```
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860562876     A.U. after   10 cycles
             Convg  =    0.8009D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6          -0.000106736   -0.000083787    0.000004576
      2          6           0.000174022   -0.000167305   -0.000008733
      3          6           0.000211363   -0.000036968   -0.000017075
      4          6          -0.000086715    0.000148573    0.000006665
      5          6          -0.000165973    0.000030471   -0.000004994
      6          6          -0.000103016    0.000095750    0.000004919
      7          6           0.000022315   -0.000055798    0.000033966
      8          6           0.000167342   -0.000350943    0.000038467
      9          6          -0.000048351    0.000135606    0.000010510
     10          6          -0.000071484   -0.000175889   -0.000014617
     11          6           0.000055575   -0.000239392   -0.000012450
     12          1          -0.000004429    0.000144944    0.000003886
     13          6           0.000123610    0.000062070    0.000007199
     14          6          -0.000024938    0.000132192    0.000005737
     15          6           0.000022581    0.000162269   -0.000005596
     16          1          -0.000056392    0.000094543   -0.000026721
     17          1           0.000067070    0.000065780    0.000000369
     18          1          -0.000124082    0.000074914    0.000000776
     19          1           0.000091365   -0.000030323    0.000000098
     20          1           0.000105064   -0.000019609    0.000008725
     21          1          -0.000090146   -0.000025621   -0.000002277
     22          1          -0.000032687   -0.000101663    0.000008541
     23          1          -0.000041438   -0.000091061   -0.000002800
     24          6          -0.000353713    0.000586430    0.000065606
     25          1           0.000077880   -0.000120818    0.000186331
     26          1           0.000250152   -0.000030290   -0.000156953
     27          1          -0.000058240   -0.000204075   -0.000134152
```

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000586430 RMS     0.000128377


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000245326 RMS     0.000070522
 Search for a local minimum.
 Step number  11 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
11
                                                      9
 DE=  2.46D-06 DEPred=-3.97D-07 R=-6.20D+00
 Trust test=-6.20D+00 RLast= 5.15D-02 DXMaxT set to 1.26D-01
 Use linear search instead of GDIIS.
 Quartic linear search produced a step of -0.93657.
 Iteration  1 RMS(Cart)=  0.00594518 RMS(Int)=  0.00004942
 Iteration  2 RMS(Cart)=  0.00005127 RMS(Int)=  0.00000003
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000003
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.58923   0.00008   0.00028   0.00000   0.00028
2.58952
    R2        2.69187   0.00007   0.00012   0.00000   0.00012
2.69198
    R3        2.05421  -0.00009  -0.00025   0.00000  -0.00025
2.05395
    R4        2.70500   0.00007   0.00011   0.00000   0.00011
2.70511
    R5        2.05627  -0.00013  -0.00040   0.00000  -0.00040
2.05588
    R6        2.73534   0.00015   0.00021   0.00000   0.00021
2.73555
    R7        2.64202  -0.00003  -0.00009   0.00000  -0.00009
2.64193
    R8        2.71272   0.00003  -0.00002   0.00000  -0.00002
2.71271
    R9        2.67969  -0.00008  -0.00030   0.00000  -0.00030
2.67939
   R10        2.59477  -0.00004  -0.00008   0.00000  -0.00008
2.59469
   R11        2.04889  -0.00008  -0.00017   0.00000  -0.00017
2.04872
   R12        2.05470  -0.00010  -0.00031   0.00000  -0.00031
2.05438
```

R13	2.64202	-0.00003	-0.00014	0.00000	-0.00014
2.64188					
R14	2.05733	-0.00011	-0.00033	0.00000	-0.00033
2.05700					
R15	2.67962	-0.00011	-0.00021	0.00000	-0.00021
2.67942					
R16	2.86066	0.00024	0.00174	0.00000	0.00174
2.86240					
R17	2.73521	0.00011	0.00065	0.00000	0.00065
2.73586					
R18	2.71266	0.00000	0.00018	0.00000	0.00018
2.71284					
R19	2.70497	0.00007	0.00020	0.00000	0.00020
2.70517					
R20	2.05628	-0.00013	-0.00040	0.00000	-0.00040
2.05588					
R21	2.58927	0.00010	0.00017	0.00000	0.00017
2.58944					
R22	2.69187	0.00007	0.00012	0.00000	0.00012
2.69199					
R23	2.05421	-0.00009	-0.00026	0.00000	-0.00026
2.05395					
R24	2.59479	-0.00004	-0.00017	0.00000	-0.00017
2.59463					
R25	2.05470	-0.00010	-0.00031	0.00000	-0.00031
2.05438					
R26	2.04893	-0.00006	-0.00028	0.00000	-0.00028
2.04865					
R27	2.07756	0.00012	0.00015	0.00000	0.00015
2.07771					
R28	2.06417	0.00018	0.00004	0.00000	0.00004
2.06421					
R29	2.06398	0.00013	0.00063	0.00000	0.00063
2.06461					
A1	2.08874	0.00005	0.00049	0.00000	0.00049
2.08922					
A2	2.10305	-0.00005	-0.00052	0.00000	-0.00052
2.10253					
A3	2.09139	0.00000	0.00003	0.00000	0.00003
2.09143					
A4	2.11656	-0.00003	-0.00021	0.00000	-0.00021
2.11635					
A5	2.10492	-0.00005	-0.00062	0.00000	-0.00062
2.10430					
A6	2.06169	0.00008	0.00082	0.00000	0.00082
2.06251					
A7	2.08580	-0.00007	-0.00048	0.00000	-0.00048
2.08532					
A8	2.11099	0.00005	0.00061	0.00000	0.00061
2.11160					
A9	2.08639	0.00002	-0.00013	0.00000	-0.00013
2.08626					

This journal is © The Royal Society of Chemistry 2014

A10	2.04255	0.00007	0.00072	0.00000	0.00072
2.04327					
A11	2.09312	-0.00005	0.00001	0.00000	0.00001
2.09313					
A12	2.14747	-0.00002	-0.00073	0.00000	-0.00073
2.14674					
A13	2.12488	-0.00002	-0.00031	0.00000	-0.00031
2.12457					
A14	2.08865	-0.00005	-0.00074	0.00000	-0.00074
2.08791					
A15	2.06957	0.00007	0.00104	0.00000	0.00104
2.07061					
A16	2.10769	0.00000	-0.00021	0.00000	-0.00021
2.10748					
A17	2.08631	-0.00002	-0.00021	0.00000	-0.00021
2.08609					
A18	2.08918	0.00002	0.00042	0.00000	0.00042
2.08961					
A19	2.11907	-0.00002	-0.00002	0.00000	-0.00002
2.11905					
A20	2.08202	0.00001	0.00004	0.00000	0.00004
2.08206					
A21	2.08204	0.00001	-0.00002	0.00000	-0.00002
2.08202					
A22	2.08744	0.00006	0.00037	0.00000	0.00037
2.08780					
A23	2.09826	0.00006	-0.00156	0.00000	-0.00156
2.09670					
A24	2.09735	-0.00012	0.00121	0.00000	0.00121
2.09857					
A25	2.09331	-0.00001	-0.00055	0.00000	-0.00055
2.09276					
A26	2.14714	-0.00010	0.00026	0.00000	0.00026
2.14740					
A27	2.04269	0.00011	0.00029	0.00000	0.00029
2.04298					
A28	2.08626	0.00000	0.00023	0.00000	0.00023
2.08650					
A29	2.11116	0.00008	0.00012	0.00000	0.00012
2.11128					
A30	2.08575	-0.00008	-0.00035	0.00000	-0.00035
2.08540					
A31	2.06172	0.00009	0.00072	0.00000	0.00072
2.06244					
A32	2.11653	-0.00004	-0.00010	0.00000	-0.00010
2.11643					
A33	2.10492	-0.00005	-0.00061	0.00000	-0.00061
2.10430					
A34	2.08878	0.00006	0.00035	0.00000	0.00035
2.08913					
A35	2.10302	-0.00006	-0.00044	0.00000	-0.00044
2.10258					

This journal is © The Royal Society of Chemistry 2014

A36	2.09138	0.00000	0.00009	0.00000	0.00009	2.09147
A37	2.10766	-0.00001	-0.00010	0.00000	-0.00010	2.10756
A38	2.08631	-0.00002	-0.00022	0.00000	-0.00022	2.08609
A39	2.08922	0.00003	0.00032	0.00000	0.00032	2.08953
A40	2.12481	-0.00004	-0.00009	0.00000	-0.00009	2.12472
A41	2.08854	-0.00006	-0.00044	0.00000	-0.00044	2.08810
A42	2.06975	0.00010	0.00052	0.00000	0.00052	2.07026
A43	1.95110	-0.00017	-0.00109	0.00000	-0.00109	1.95002
A44	1.95398	-0.00025	-0.00137	0.00000	-0.00137	1.95262
A45	1.95455	-0.00020	-0.00309	0.00000	-0.00309	1.95146
A46	1.87159	0.00024	0.00246	0.00000	0.00246	1.87405
A47	1.87170	0.00023	0.00215	0.00000	0.00215	1.87385
A48	1.85529	0.00020	0.00139	0.00000	0.00139	1.85667
D1	-0.00160	0.00001	0.00024	0.00000	0.00024	-0.00136
D2	3.13492	0.00000	-0.00014	0.00000	-0.00014	3.13479
D3	-3.13883	0.00001	0.00037	0.00000	0.00037	-3.13846
D4	-0.00231	0.00000	-0.00001	0.00000	-0.00001	-0.00232
D5	0.00881	0.00000	0.00044	0.00000	0.00044	0.00925
D6	-3.13044	0.00001	0.00062	0.00000	0.00062	-3.12982
D7	-3.13711	0.00000	0.00031	0.00000	0.00031	-3.13680
D8	0.00682	0.00000	0.00050	0.00000	0.00050	0.00732
D9	-0.01214	-0.00001	-0.00069	0.00000	-0.00069	-0.01283
D10	3.12565	-0.00001	-0.00080	0.00000	-0.00080	3.12485
D11	3.13440	0.00000	-0.00032	0.00000	-0.00032	3.13409
D12	-0.01099	0.00000	-0.00043	0.00000	-0.00043	-0.01143
D13	0.01823	0.00000	0.00047	0.00000	0.00047	0.01870

This journal is © The Royal Society of Chemistry 2014

D14	-3.13254	0.00000	0.00037	0.00000	0.00037	-3.13217
D15	-3.11961	0.00000	0.00058	0.00000	0.00058	-3.11903
D16	0.01280	0.00001	0.00049	0.00000	0.00049	0.01329
D17	-3.12313	0.00001	0.00108	0.00000	0.00108	-3.12205
D18	0.00751	0.00001	0.00132	0.00000	0.00132	0.00883
D19	0.01466	0.00001	0.00096	0.00000	0.00096	0.01562
D20	-3.13788	0.00001	0.00121	0.00000	0.00121	-3.13668
D21	-0.01149	0.00001	0.00019	0.00000	0.00019	-0.01130
D22	3.11575	0.00000	-0.00053	0.00000	-0.00053	3.11523
D23	3.13960	0.00000	0.00029	0.00000	0.00029	3.13988
D24	-0.01635	-0.00001	-0.00043	0.00000	-0.00043	-0.01678
D25	-0.03968	-0.00002	-0.00201	0.00000	-0.00201	-0.04169
D26	3.11992	-0.00003	-0.00348	0.00000	-0.00348	3.11643
D27	3.09215	-0.00002	-0.00210	0.00000	-0.00210	3.09005
D28	-0.03143	-0.00003	-0.00358	0.00000	-0.00358	-0.03501
D29	-0.00194	-0.00001	-0.00066	0.00000	-0.00066	-0.00259
D30	3.13731	-0.00001	-0.00084	0.00000	-0.00084	3.13647
D31	-3.12933	0.00000	0.00007	0.00000	0.00007	-3.12926
D32	0.00992	0.00000	-0.00011	0.00000	-0.00011	0.00981
D33	-0.01469	-0.00001	-0.00088	0.00000	-0.00088	-0.01556
D34	3.12309	-0.00001	-0.00101	0.00000	-0.00101	3.12208
D35	3.13786	-0.00001	-0.00112	0.00000	-0.00112	3.13674
D36	-0.00755	-0.00001	-0.00126	0.00000	-0.00126	-0.00881
D37	0.03966	0.00002	0.00208	0.00000	0.00208	0.04174
D38	-3.09219	0.00001	0.00219	0.00000	0.00219	-3.09000
D39	-3.11993	0.00003	0.00353	0.00000	0.00353	-3.11640

This journal is © The Royal Society of Chemistry 2014

D40	0.03140	0.00003	0.00364	0.00000	0.00364	0.03504
D41	1.56962	0.00002	-0.01889	0.00000	-0.01889	1.55073
D42	-2.61318	0.00003	-0.01745	0.00000	-0.01745	-2.63063
D43	-0.53130	-0.00002	-0.01873	0.00000	-0.01873	-0.55004
D44	-1.55386	0.00000	-0.02037	0.00000	-0.02037	-1.57423
D45	0.54652	0.00001	-0.01892	0.00000	-0.01892	0.52760
D46	2.62840	-0.00004	-0.02021	0.00000	-0.02021	2.60819
D47	-0.01275	0.00000	-0.00066	0.00000	-0.00066	-0.01340
D48	3.13261	0.00000	-0.00052	0.00000	-0.00052	3.13208
D49	3.11968	0.00000	-0.00076	0.00000	-0.00076	3.11892
D50	-0.01815	0.00000	-0.00063	0.00000	-0.00063	-0.01878
D51	-3.13967	0.00000	-0.00013	0.00000	-0.00013	-3.13980
D52	0.01623	0.00000	0.00070	0.00000	0.00070	0.01693
D53	0.01139	-0.00001	-0.00001	0.00000	-0.00001	0.01138
D54	-3.11588	0.00000	0.00081	0.00000	0.00081	-3.11507
D55	0.01104	0.00000	0.00042	0.00000	0.00042	0.01146
D56	-3.12565	0.00001	0.00087	0.00000	0.00087	-3.12478
D57	-3.13437	0.00000	0.00028	0.00000	0.00028	-3.13408
D58	0.01212	0.00001	0.00074	0.00000	0.00074	0.01286
D59	0.00156	-0.00001	-0.00018	0.00000	-0.00018	0.00138
D60	3.13878	-0.00001	-0.00031	0.00000	-0.00031	3.13846
D61	-3.13502	0.00000	0.00028	0.00000	0.00028	-3.13474
D62	0.00220	0.00000	0.00015	0.00000	0.00015	0.00235
D63	-0.00879	0.00000	-0.00048	0.00000	-0.00048	-0.00927
D64	3.13049	0.00000	-0.00073	0.00000	-0.00073	3.12976
D65	3.13715	0.00000	-0.00035	0.00000	-0.00035	3.13680

```
   D66       -0.00676   0.00000  -0.00060   0.00000  -0.00060  -
0.00735
   D67        0.00198   0.00001   0.00058   0.00000   0.00058
0.00255
   D68        3.12941   0.00000  -0.00025   0.00000  -0.00025
3.12916
   D69       -3.13729   0.00001   0.00082   0.00000   0.00082  -
3.13647
   D70       -0.00987   0.00000  -0.00001   0.00000  -0.00001  -
0.00987
         Item               Value     Threshold  Converged?
 Maximum Force            0.000245     0.000450     YES
 RMS     Force            0.000071     0.000300     YES
 Maximum Displacement     0.041460     0.001800     NO
 RMS     Displacement     0.005947     0.001200     NO
 Predicted change in Energy=-1.734657D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792003   -5.432486    0.005783
      2          6           0       -3.422409   -5.398231   -0.022447
      3          6           0       -2.710519   -4.156366   -0.033508
      4          6           0       -3.449462   -2.911588   -0.030715
      5          6           0       -4.881605   -3.002120    0.007185
      6          6           0       -5.528324   -4.213177    0.026291
      7          6           0       -1.312786   -4.128033   -0.042262
      8          6           0       -2.754132   -1.676122   -0.053176
      9          6           0       -1.336507   -1.669189   -0.026888
     10          6           0       -0.608369   -2.920510   -0.029777
     11          6           0        0.822957   -2.902844   -0.014947
     12          1           0        1.348462   -3.855381   -0.024642
     13          6           0        1.519271   -1.723113    0.017024
     14          6           0        0.812223   -0.486597    0.037725
     15          6           0       -0.560391   -0.462226    0.015078
     16          1           0       -0.761097   -5.066365   -0.048998
     17          1           0       -5.319386   -6.382807    0.016822
     18          1           0       -2.845968   -6.320838   -0.031990
     19          1           0       -5.475389   -2.095495    0.035499
     20          1           0       -6.614510   -4.243770    0.059806
     21          1           0        2.606086   -1.724807    0.030898
     22          1           0        1.367343    0.447408    0.074266
     23          1           0       -1.063209    0.497785    0.043773
     24          6           0       -3.522916   -0.371348   -0.083314
     25          1           0       -3.751512   -0.010127    0.929659
     26          1           0       -2.965538    0.417796   -0.592995
     27          1           0       -4.471737   -0.471462   -0.615634
```

This journal is © The Royal Society of Chemistry 2014

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370313	0.000000			
3	C	2.441844	1.431481	0.000000		
4	C	2.856339	2.486804	1.447590	0.000000	
5	C	2.432018	2.805616	2.459178	1.435502	0.000000
6	C	1.424537	2.416941	2.819012	2.453375	1.373052
7	C	3.716028	2.462582	1.398048	2.458711	3.742539
8	C	4.273953	3.781751	2.480706	1.417874	2.507600
9	C	5.109200	4.272793	2.841479	2.451153	3.787557
10	C	4.879968	3.749397	2.438522	2.841107	4.274175
11	C	6.158514	4.924444	3.749282	4.272458	5.705469
12	H	6.339835	5.014141	4.070135	4.889874	6.288308
13	C	7.320639	6.158592	4.880000	5.109116	6.527417
14	C	7.474637	6.485359	5.087435	4.903797	6.224827
15	C	6.527642	5.705848	4.274585	3.787902	5.012386
16	H	4.047869	2.682056	2.151414	3.445389	4.608997
17	H	1.086905	2.137627	3.430125	3.943124	3.408928
18	H	2.139544	1.087924	2.168706	3.462252	3.893488
19	H	3.406378	3.889235	3.449125	2.185125	1.084135
20	H	2.176580	3.395446	3.906085	3.435175	2.132469
21	H	8.275218	7.059719	5.846615	6.171054	7.595894
22	H	8.515597	7.557948	6.151041	5.873286	7.138143
23	H	7.005245	6.350844	4.937684	4.162160	5.179847
24	C	5.218586	5.028256	3.871541	2.541846	2.962293
25	H	5.598049	5.481467	4.382084	3.071161	3.328677
26	H	6.157947	5.861777	4.615303	3.411032	3.965773
27	H	5.010039	5.072082	4.125443	2.709500	2.638204

		6	7	8	9	10
6	C	0.000000				
7	C	4.216956	0.000000			
8	C	3.760201	2.844199	0.000000		
9	C	4.903676	2.459006	1.417886	0.000000	
10	C	5.087248	1.398024	2.480594	1.447755	0.000000
11	C	6.485172	2.462363	3.781782	2.487033	1.431512
12	H	6.886277	2.675237	4.645564	3.462441	2.168686
13	C	7.474564	3.715872	4.274238	2.856625	2.441885
14	C	7.354595	4.216884	3.760601	2.453516	2.818966
15	C	6.224959	3.742662	2.508126	1.435575	2.459160
16	H	4.843558	1.088519	3.932678	3.445633	2.151370
17	H	2.179687	4.597863	5.360813	6.171177	5.846653
18	H	3.411842	2.675659	4.645673	4.890433	4.070515
19	H	2.118364	4.632982	2.754810	4.161247	4.936881
20	H	1.087134	5.303970	4.637683	5.873099	6.150835
21	H	8.506505	4.597651	5.361098	3.943408	3.430175
22	H	8.323075	5.303897	4.638122	3.435261	3.906038
23	H	6.490818	4.633344	2.755810	2.185283	3.449206
24	C	4.335127	4.358789	1.514718	2.543218	3.872425
25	H	4.651749	4.883561	2.176297	3.082161	4.389782
26	H	5.328912	4.868208	2.172691	2.707346	4.125256

This journal is © The Royal Society of Chemistry 2014

27	H	3.940669	4.866029	2.172034	3.407468	4.611581
		11	12	13	14	15
11	C	0.000000				
12	H	1.087923	0.000000			
13	C	1.370270	2.139504	0.000000		
14	C	2.416845	3.411766	1.424541	0.000000	
15	C	2.805560	3.893430	2.432043	1.373018	0.000000
16	H	2.681644	2.432554	4.047441	4.843256	4.608957
17	H	7.059712	7.130905	8.275263	8.506606	7.596137
18	H	5.014378	4.865366	6.340094	6.886624	6.288832
19	H	6.350081	7.047394	7.004590	6.490195	5.179304
20	H	7.557751	7.972886	8.515512	8.323052	7.138237
21	H	2.137620	2.474681	1.086904	2.179714	3.408950
22	H	3.395365	4.303967	2.176584	1.087133	2.132392
23	H	3.889132	4.977036	3.406216	2.118086	1.084099
24	C	5.029887	5.989345	5.221206	4.338360	2.965551
25	H	5.494166	6.458050	5.616794	4.674425	3.350239
26	H	5.070846	6.098660	5.006907	3.935379	2.632284
27	H	5.857152	6.758321	6.152972	5.324222	3.961882
		16	17	18	19	20
16	H	0.000000				
17	H	4.745034	0.000000			
18	H	2.433245	2.474675	0.000000		
19	H	5.572949	4.290190	4.977141	0.000000	
20	H	5.911933	2.500935	4.304016	2.431722	0.000000
21	H	4.744503	9.192946	7.131083	8.089973	9.558525
22	H	5.911611	9.558633	7.973232	7.300057	9.258366
23	H	5.573118	8.090631	7.048233	5.117861	7.300653
24	C	5.447202	6.274947	5.988098	2.607479	4.957225
25	H	5.955325	6.625900	6.447469	2.849568	5.184316
26	H	5.935614	7.222235	6.763003	3.607075	5.955782
27	H	5.933217	6.005206	6.099096	2.017120	4.390672
		21	22	23	24	25
21	H	0.000000				
22	H	2.500977	0.000000			
23	H	4.289966	2.431265	0.000000		
24	C	6.277703	4.960829	2.611839	0.000000	
25	H	6.645821	5.209962	2.875715	1.099478	0.000000
26	H	6.001914	4.384058	2.007667	1.092334	1.766168
27	H	7.216956	5.951062	3.604487	1.092542	1.766206
		26	27			
26	H	0.000000				
27	H	1.749266	0.000000			

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.660040	-0.994497	0.021793
2	6	0	-2.461904	-1.658684	-0.011152
3	6	0	-1.219004	-0.948586	-0.021082
4	6	0	-1.225474	0.498961	-0.012050
5	6	0	-2.506033	1.146274	0.030620
6	6	0	-3.677125	0.429687	0.048457
7	6	0	0.000423	-1.632217	-0.034668
8	6	0	-0.000110	1.211981	-0.033341
9	6	0	1.225679	0.499670	-0.012017
10	6	0	1.219518	-0.948043	-0.021126
11	6	0	2.462540	-1.657992	-0.011277
12	1	0	2.433032	-2.745420	-0.025607
13	6	0	3.660600	-0.993758	0.021697
14	6	0	3.677471	0.430431	0.048501
15	6	0	2.506353	1.146912	0.030752
16	1	0	0.000690	-2.720676	-0.046088
17	1	0	-4.596163	-1.546707	0.031906
18	1	0	-2.432333	-2.746112	-0.025420
19	1	0	-2.558624	2.228629	0.063674
20	1	0	-4.629050	0.953433	0.085701
21	1	0	4.596783	-1.545863	0.031744
22	1	0	4.629315	0.954317	0.085822
23	1	0	2.559237	2.229209	0.064023
24	6	0	-0.001965	2.726514	-0.056958
25	1	0	-0.014484	3.149396	0.957865
26	1	0	0.877593	3.126712	-0.566285
27	1	0	-0.871555	3.123166	-0.586229

```
 Rotational constants (GHZ):      1.3930723      0.4479083
0.3397516
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8809102901 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
       Virtual  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860565352     A.U. after   10 cycles
             Convg  =    0.8478D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
```

```
 ---------------------------------------------------------------------
      1        6           0.000010642   -0.000002317   -0.000001539
      2        6          -0.000016455    0.000014163    0.000001358
      3        6          -0.000027289    0.000005113    0.000005008
      4        6           0.000012692   -0.000012279    0.000005727
      5        6           0.000017950   -0.000001613   -0.000003080
      6        6           0.000008645   -0.000000238    0.000001451
      7        6           0.000003848    0.000004253   -0.000006122
      8        6          -0.000001478    0.000041377   -0.000008911
      9        6          -0.000016395   -0.000011239   -0.000004686
     10        6           0.000004697    0.000013428    0.000004613
     11        6           0.000000102    0.000024097    0.000001735
     12        1          -0.000002579   -0.000013267    0.000000673
     13        6          -0.000001275   -0.000015967   -0.000002241
     14        6          -0.000009810   -0.000005386    0.000001420
     15        6           0.000004447   -0.000020214   -0.000003336
     16        1           0.000004838   -0.000007450    0.000005650
     17        1          -0.000006685   -0.000002811    0.000001200
     18        1           0.000011974   -0.000004605    0.000001154
     19        1          -0.000008858    0.000006012   -0.000001151
     20        1          -0.000008449    0.000001591   -0.000002034
     21        1           0.000005655    0.000004162    0.000001577
     22        1           0.000002244    0.000008277   -0.000002411
     23        1           0.000004914    0.000010721   -0.000000751
     24        6           0.000050482   -0.000071851    0.000002485
     25        1          -0.000013243    0.000011372   -0.000013517
     26        1          -0.000025135    0.000008253    0.000015816
     27        1          -0.000005478    0.000016418   -0.000000088
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000071851 RMS     0.000014271


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000034271 RMS     0.000008027
 Search for a local minimum.
 Step number  12 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12
     Eigenvalues ---   -0.00994   0.00000   0.01506   0.01765
0.01788
     Eigenvalues ---    0.01814   0.01819   0.01829   0.01962
0.01970
```

```
     Eigenvalues ---    0.01977   0.02011   0.02029   0.02055
0.02111
     Eigenvalues ---    0.02125   0.02146   0.02172   0.02226
0.02264
     Eigenvalues ---    0.02346   0.02483   0.04259   0.06825
0.07057
     Eigenvalues ---    0.12656   0.15817   0.15985   0.15999
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16015   0.16051
0.16175
     Eigenvalues ---    0.16231   0.20350   0.21997   0.22168
0.22608
     Eigenvalues ---    0.23349   0.23756   0.24459   0.24994
0.25133
     Eigenvalues ---    0.27971   0.31386   0.33208   0.33587
0.33631
     Eigenvalues ---    0.33681   0.33682   0.33682   0.33823
0.34017
     Eigenvalues ---    0.34173   0.35848   0.36966   0.37245
0.37569
     Eigenvalues ---    0.38021   0.38517   0.39442   0.39892
0.40484
     Eigenvalues ---    0.41174   0.41521   0.44391   0.44724
0.45391
     Eigenvalues ---    0.49636   0.49834   0.50017   0.51311
0.56186
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is  -9.94D-03 should be greater than     0.000000
Eigenvector:
                          D28       A48       D40       D26       D39
   1                    0.27789   0.26938  -0.25816   0.25200  -
0.24706
                          D46       A44       D27       R16       D44
   1                    0.21752  -0.18317   0.18097   0.17846
0.16796
 Eigenvalue     2 is   3.61D-06 Eigenvector:
                          D41       D42       D43       D44       D45
   1                    0.41969   0.41961   0.38685   0.38684
0.38676
                          D46       D28       D40       D26       D39
   1                    0.35400  -0.09045   0.08515  -0.08176
0.07904
 Use linear search instead of GDIIS.
 RFO step:  Lambda=-1.22662470D-06 EMin= 9.94139729D-03
 Quartic linear search produced a step of  0.00092.
 Iteration  1 RMS(Cart)=  0.01270606 RMS(Int)=  0.00021591
 Iteration  2 RMS(Cart)=  0.00022495 RMS(Int)=  0.00000125
 Iteration  3 RMS(Cart)=  0.00000006 RMS(Int)=  0.00000125
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58952  -0.00001   0.00000  -0.00013  -0.00013
2.58938
    R2        2.69198   0.00000   0.00000  -0.00019  -0.00019
2.69180
    R3        2.05395   0.00001   0.00000   0.00010   0.00010
2.05405
    R4        2.70511  -0.00001   0.00000   0.00016   0.00016
2.70527
    R5        2.05588   0.00001   0.00000  -0.00018  -0.00018
2.05570
    R6        2.73555  -0.00002   0.00000  -0.00028  -0.00028
2.73527
    R7        2.64193   0.00001   0.00000   0.00025   0.00025
2.64218
    R8        2.71271  -0.00001   0.00000   0.00067   0.00067
2.71338
    R9        2.67939   0.00000   0.00000   0.00192   0.00192
2.68131
   R10        2.59469   0.00000   0.00000   0.00069   0.00069
2.59538
   R11        2.04872   0.00001   0.00000  -0.00037  -0.00037
2.04835
   R12        2.05438   0.00001   0.00000  -0.00057  -0.00057
2.05382
```

R13	2.64188	0.00000	0.00000	0.00011	0.00011
2.64199					
R14	2.05700	0.00001	0.00000	-0.00026	-0.00026
2.05675					
R15	2.67942	-0.00001	0.00000	0.00213	0.00213
2.68154					
R16	2.86240	-0.00003	0.00000	0.00263	0.00263
2.86503					
R17	2.73586	-0.00001	0.00000	0.00075	0.00075
2.73661					
R18	2.71284	0.00000	0.00000	0.00124	0.00124
2.71409					
R19	2.70517	0.00000	0.00000	0.00032	0.00032
2.70549					
R20	2.05588	0.00001	0.00000	-0.00018	-0.00018
2.05569					
R21	2.58944	-0.00001	0.00000	-0.00043	-0.00043
2.58901					
R22	2.69199	0.00000	0.00000	-0.00017	-0.00017
2.69182					
R23	2.05395	0.00001	0.00000	0.00010	0.00010
2.05405					
R24	2.59463	0.00000	0.00000	0.00051	0.00051
2.59513					
R25	2.05438	0.00001	0.00000	-0.00058	-0.00058
2.05381					
R26	2.04865	0.00001	0.00000	-0.00063	-0.00063
2.04802					
R27	2.07771	-0.00001	0.00000	-0.00124	-0.00124
2.07647					
R28	2.06421	-0.00001	0.00000	-0.00197	-0.00197
2.06224					
R29	2.06461	0.00000	0.00000	-0.00082	-0.00082
2.06379					
A1	2.08922	-0.00001	0.00000	0.00132	0.00132
2.09054					
A2	2.10253	0.00001	0.00000	-0.00139	-0.00139
2.10113					
A3	2.09143	0.00000	0.00000	0.00008	0.00008
2.09150					
A4	2.11635	0.00000	0.00000	-0.00065	-0.00065
2.11570					
A5	2.10430	0.00001	0.00000	-0.00013	-0.00013
2.10418					
A6	2.06251	-0.00001	0.00000	0.00078	0.00078
2.06329					
A7	2.08532	0.00001	0.00000	-0.00042	-0.00042
2.08490					
A8	2.11160	0.00000	0.00000	0.00030	0.00030
2.11190					
A9	2.08626	-0.00001	0.00000	0.00012	0.00012
2.08637					

This journal is © The Royal Society of Chemistry 2014

A10	2.04327	0.00000	0.00000	0.00129	0.00129
2.04456					
A11	2.09313	0.00001	0.00000	-0.00014	-0.00014
2.09300					
A12	2.14674	-0.00001	0.00000	-0.00114	-0.00114
2.14560					
A13	2.12457	0.00000	0.00000	-0.00110	-0.00110
2.12347					
A14	2.08791	0.00000	0.00000	-0.00088	-0.00089
2.08702					
A15	2.07061	0.00000	0.00000	0.00203	0.00203
2.07264					
A16	2.10748	0.00000	0.00000	-0.00040	-0.00040
2.10709					
A17	2.08609	0.00000	0.00000	0.00022	0.00022
2.08631					
A18	2.08961	0.00000	0.00000	0.00018	0.00018
2.08979					
A19	2.11905	0.00000	0.00000	0.00028	0.00028
2.11934					
A20	2.08206	0.00000	0.00000	-0.00013	-0.00013
2.08193					
A21	2.08202	0.00000	0.00000	-0.00015	-0.00015
2.08187					
A22	2.08780	0.00000	0.00000	0.00040	0.00040
2.08820					
A23	2.09670	-0.00003	0.00000	-0.00322	-0.00322
2.09348					
A24	2.09857	0.00003	0.00000	0.00277	0.00277
2.10133					
A25	2.09276	0.00000	0.00000	-0.00132	-0.00132
2.09144					
A26	2.14740	0.00001	0.00000	0.00102	0.00103
2.14843					
A27	2.04298	-0.00001	0.00000	0.00030	0.00030
2.04328					
A28	2.08650	0.00000	0.00000	0.00084	0.00084
2.08734					
A29	2.11128	-0.00001	0.00000	-0.00070	-0.00070
2.11058					
A30	2.08540	0.00001	0.00000	-0.00014	-0.00014
2.08526					
A31	2.06244	-0.00001	0.00000	0.00054	0.00054
2.06298					
A32	2.11643	0.00000	0.00000	-0.00039	-0.00039
2.11604					
A33	2.10430	0.00001	0.00000	-0.00015	-0.00015
2.10415					
A34	2.08913	-0.00001	0.00000	0.00105	0.00105
2.09018					
A35	2.10258	0.00001	0.00000	-0.00122	-0.00122
2.10136					

This journal is © The Royal Society of Chemistry 2014

A36	2.09147	0.00000	0.00000	0.00017	0.00017	2.09164
A37	2.10756	0.00000	0.00000	-0.00018	-0.00018	2.10738
A38	2.08609	0.00000	0.00000	0.00023	0.00023	2.08632
A39	2.08953	0.00000	0.00000	-0.00005	-0.00005	2.08948
A40	2.12472	0.00001	0.00000	-0.00061	-0.00061	2.12412
A41	2.08810	0.00001	0.00000	-0.00025	-0.00025	2.08785
A42	2.07026	-0.00001	0.00000	0.00089	0.00089	2.07116
A43	1.95002	0.00002	0.00000	0.00019	0.00018	1.95020
A44	1.95262	0.00003	0.00000	-0.00017	-0.00018	1.95244
A45	1.95146	0.00001	0.00000	-0.00382	-0.00383	1.94764
A46	1.87405	-0.00002	0.00000	0.00024	0.00024	1.87429
A47	1.87385	-0.00002	0.00000	-0.00057	-0.00057	1.87329
A48	1.85667	-0.00002	0.00000	0.00445	0.00445	1.86112
D1	-0.00136	0.00000	0.00000	-0.00010	-0.00010	-0.00146
D2	3.13479	0.00000	0.00000	0.00025	0.00025	3.13504
D3	-3.13846	0.00000	0.00000	-0.00136	-0.00136	-3.13982
D4	-0.00232	0.00000	0.00000	-0.00100	-0.00100	-0.00332
D5	0.00925	0.00000	0.00000	-0.00212	-0.00212	0.00713
D6	-3.12982	0.00000	0.00000	-0.00168	-0.00168	-3.13150
D7	-3.13680	0.00000	0.00000	-0.00088	-0.00088	-3.13768
D8	0.00732	0.00000	0.00000	-0.00043	-0.00043	0.00688
D9	-0.01283	0.00000	0.00000	0.00258	0.00258	-0.01025
D10	3.12485	0.00000	0.00000	0.00245	0.00245	3.12729
D11	3.13409	0.00000	0.00000	0.00224	0.00224	3.13632
D12	-0.01143	0.00000	0.00000	0.00210	0.00210	-0.00932
D13	0.01870	0.00000	0.00000	-0.00279	-0.00279	0.01591

D14	-3.13217	0.00000	0.00000	-0.00203	-0.00203	-3.13420
D15	-3.11903	0.00000	0.00000	-0.00266	-0.00266	-3.12169
D16	0.01329	0.00000	0.00000	-0.00190	-0.00190	0.01139
D17	-3.12205	0.00000	0.00000	-0.00129	-0.00129	-3.12334
D18	0.00883	0.00000	0.00000	-0.00119	-0.00119	0.00765
D19	0.01562	0.00000	0.00000	-0.00142	-0.00142	0.01420
D20	-3.13668	0.00000	0.00000	-0.00132	-0.00132	-3.13800
D21	-0.01130	0.00000	0.00000	0.00065	0.00065	-0.01065
D22	3.11523	0.00000	0.00000	0.00433	0.00433	3.11955
D23	3.13988	0.00000	0.00000	-0.00014	-0.00014	3.13974
D24	-0.01678	0.00000	0.00000	0.00354	0.00354	-0.01324
D25	-0.04169	0.00000	0.00000	0.00480	0.00480	-0.03689
D26	3.11643	0.00001	0.00000	0.00802	0.00801	3.12445
D27	3.09005	0.00000	0.00000	0.00562	0.00562	3.09567
D28	-0.03501	0.00001	0.00000	0.00884	0.00883	-0.02618
D29	-0.00259	0.00000	0.00000	0.00182	0.00182	-0.00077
D30	3.13647	0.00000	0.00000	0.00137	0.00137	3.13784
D31	-3.12926	0.00000	0.00000	-0.00180	-0.00181	-3.13107
D32	0.00981	0.00000	0.00000	-0.00225	-0.00225	0.00755
D33	-0.01556	0.00000	0.00000	0.00177	0.00177	-0.01380
D34	3.12208	0.00000	0.00000	0.00135	0.00135	3.12342
D35	3.13674	0.00000	0.00000	0.00167	0.00167	3.13841
D36	-0.00881	0.00000	0.00000	0.00125	0.00125	-0.00756
D37	0.04174	0.00000	0.00000	-0.00447	-0.00447	0.03727
D38	-3.09000	0.00000	0.00000	-0.00513	-0.00513	-3.09513
D39	-3.11640	-0.00001	0.00000	-0.00776	-0.00776	-3.12416

This journal is © The Royal Society of Chemistry 2014

D40	0.03504	-0.00001	0.00000	-0.00841	-0.00842	0.02663
D41	1.55073	-0.00001	-0.00002	-0.04299	-0.04300	1.50773
D42	-2.63063	-0.00001	-0.00002	-0.04267	-0.04269	-2.67331
D43	-0.55004	0.00000	-0.00002	-0.03973	-0.03975	-0.58979
D44	-1.57423	-0.00001	-0.00002	-0.03972	-0.03974	-1.61397
D45	0.52760	0.00000	-0.00002	-0.03941	-0.03942	0.48818
D46	2.60819	0.00000	-0.00002	-0.03647	-0.03649	2.57170
D47	-0.01340	0.00000	0.00000	0.00121	0.00121	-0.01219
D48	3.13208	0.00000	0.00000	0.00162	0.00162	3.13371
D49	3.11892	0.00000	0.00000	0.00183	0.00183	3.12075
D50	-0.01878	0.00000	0.00000	0.00224	0.00224	-0.01654
D51	-3.13980	0.00000	0.00000	0.00046	0.00046	-3.13934
D52	0.01693	0.00000	0.00000	-0.00278	-0.00278	0.01415
D53	0.01138	0.00000	0.00000	-0.00017	-0.00017	0.01121
D54	-3.11507	0.00000	0.00000	-0.00341	-0.00341	-3.11848
D55	0.01146	0.00000	0.00000	-0.00158	-0.00157	0.00989
D56	-3.12478	0.00000	0.00000	-0.00191	-0.00191	-3.12669
D57	-3.13408	0.00000	0.00000	-0.00199	-0.00199	-3.13608
D58	0.01286	0.00000	0.00000	-0.00232	-0.00232	0.01053
D59	0.00138	0.00000	0.00000	0.00025	0.00025	0.00162
D60	3.13846	0.00000	0.00000	0.00139	0.00138	3.13985
D61	-3.13474	0.00000	0.00000	-0.00010	-0.00010	-3.13483
D62	0.00235	0.00000	0.00000	0.00104	0.00104	0.00339
D63	-0.00927	0.00000	0.00000	0.00190	0.00190	-0.00737
D64	3.12976	0.00000	0.00000	0.00111	0.00111	3.13088
D65	3.13680	0.00000	0.00000	0.00077	0.00077	3.13757

```
   D66       -0.00735   0.00000   0.00000  -0.00001  -0.00001  -
0.00737
   D67        0.00255   0.00000   0.00000  -0.00192  -0.00192
0.00063
   D68        3.12916   0.00000   0.00000   0.00128   0.00128
3.13044
   D69       -3.13647   0.00000   0.00000  -0.00114  -0.00114  -
3.13761
   D70       -0.00987   0.00000   0.00000   0.00206   0.00206  -
0.00781
         Item               Value     Threshold  Converged?
 Maximum Force            0.000034     0.000450     YES
 RMS     Force            0.000008     0.000300     YES
 Maximum Displacement     0.090610     0.001800     NO
 RMS     Displacement     0.012704     0.001200     NO
 Predicted change in Energy=-1.186577D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.791864   -5.431092    0.006324
      2          6           0       -3.422238   -5.397963   -0.017996
      3          6           0       -2.710126   -4.156141   -0.030537
      4          6           0       -3.449343   -2.911696   -0.030223
      5          6           0       -4.882042   -3.000795    0.003259
      6          6           0       -5.528861   -4.212228    0.021318
      7          6           0       -1.312256   -4.127590   -0.038218
      8          6           0       -2.753634   -1.675262   -0.051687
      9          6           0       -1.334844   -1.667712   -0.027858
     10          6           0       -0.607684   -2.920063   -0.028701
     11          6           0        0.823830   -2.903510   -0.014395
     12          1           0        1.349025   -3.856135   -0.020602
     13          6           0        1.520546   -1.724151    0.012443
     14          6           0        0.815381   -0.486598    0.028541
     15          6           0       -0.557515   -0.460574    0.008767
     16          1           0       -0.760595   -5.065799   -0.041832
     17          1           0       -5.318732   -6.381759    0.017264
     18          1           0       -2.846654   -6.321028   -0.023523
     19          1           0       -5.474181   -2.093158    0.025464
     20          1           0       -6.614874   -4.243098    0.050144
     21          1           0        2.607427   -1.727564    0.024669
     22          1           0        1.371551    0.446613    0.059953
     23          1           0       -1.059733    0.499510    0.032533
     24          6           0       -3.527463   -0.371696   -0.073892
     25          1           0       -3.790214   -0.037093    0.939228
     26          1           0       -2.957880    0.431113   -0.545046
     27          1           0       -4.458459   -0.466544   -0.636877
```

This journal is © The Royal Society of Chemistry 2014

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370242	0.000000			
3	C	2.441412	1.431567	0.000000		
4	C	2.855004	2.486444	1.447440	0.000000	
5	C	2.431971	2.806758	2.460322	1.435857	0.000000
6	C	1.424437	2.417721	2.819771	2.453250	1.373415
7	C	3.716016	2.462982	1.398182	2.458781	3.743629
8	C	4.273640	3.782416	2.481350	1.418888	2.508022
9	C	5.110302	4.274586	2.843182	2.453286	3.789551
10	C	4.879944	3.749909	2.438883	2.841672	4.275240
11	C	6.158338	4.924572	3.749425	4.273210	5.706729
12	H	6.339695	5.014199	4.070234	4.890439	6.289545
13	C	7.320380	6.158647	4.880061	5.109979	6.528632
14	C	7.475942	6.486993	5.089030	4.906366	6.227556
15	C	6.529606	5.708341	4.276972	3.791067	5.015405
16	H	4.048072	2.682395	2.151343	3.445237	4.610054
17	H	1.086958	2.136770	3.429357	3.941853	3.409078
18	H	2.139326	1.087831	2.169200	3.462199	3.894543
19	H	3.407011	3.890257	3.449498	2.184737	1.083941
20	H	2.176377	3.395774	3.906549	3.435065	2.132656
21	H	8.274416	7.059073	5.846144	6.171681	7.596955
22	H	8.516923	7.559468	6.152529	5.876002	7.141097
23	H	7.007248	6.353280	4.939924	4.165393	5.182956
24	C	5.215614	5.027679	3.871943	2.541577	2.958547
25	H	5.564965	5.458078	4.367332	3.052765	3.294186
26	H	6.167086	5.871246	4.622661	3.417741	3.972534
27	H	5.017130	5.076973	4.127643	2.713874	2.647947

		6	7	8	9	10
6	C	0.000000				
7	C	4.217875	0.000000			
8	C	3.760773	2.844585	0.000000		
9	C	4.905789	2.460004	1.419011	0.000000	
10	C	5.088239	1.398082	2.480960	1.448152	0.000000
11	C	6.486194	2.462073	3.782623	2.487418	1.431681
12	H	6.887226	2.675147	4.646395	3.463004	2.169103
13	C	7.475610	3.715353	4.274941	2.856232	2.441569
14	C	7.357294	4.217596	3.762609	2.453910	2.819599
15	C	6.228109	3.744175	2.510390	1.436232	2.460286
16	H	4.844475	1.088383	3.932943	3.446295	2.151217
17	H	2.179688	4.597413	5.360559	6.172167	5.846317
18	H	3.412226	2.676895	4.646782	4.892744	4.071803
19	H	2.119779	4.632989	2.753536	4.161485	4.936547
20	H	1.086833	5.304612	4.638245	5.875152	6.151664
21	H	8.507218	4.596520	5.361860	3.943075	3.429554
22	H	8.325982	5.304318	4.640255	3.435499	3.906372
23	H	6.494128	4.634526	2.757902	2.185448	3.449866
24	C	4.331783	4.360637	1.516110	2.547422	3.875736
25	H	4.614890	4.881378	2.177156	3.102099	4.401920
26	H	5.337726	4.873062	2.173001	2.703109	4.125581

This journal is © The Royal Society of Chemistry 2014

27	H	3.950839	4.864180	2.170224	3.401570	4.606311
		11	12	13	14	15
11	C	0.000000				
12	H	1.087825	0.000000			
13	C	1.370043	2.139127	0.000000		
14	C	2.417307	3.411886	1.424449	0.000000	
15	C	2.806525	3.894302	2.432073	1.373285	0.000000
16	H	2.680793	2.431920	4.046376	4.843318	4.609978
17	H	7.059057	7.130161	8.274603	8.507666	7.598005
18	H	5.015174	4.866152	6.340742	6.888671	6.291750
19	H	6.350055	7.047436	7.004465	6.491504	5.180657
20	H	7.558636	7.973608	8.516547	8.325890	7.141483
21	H	2.136725	2.473143	1.086956	2.179780	3.409161
22	H	3.395415	4.303561	2.176390	1.086828	2.132347
23	H	3.889801	4.977608	3.406305	2.118603	1.083766
24	C	5.034617	5.993688	5.226757	4.345571	2.972427
25	H	5.514993	6.474422	5.648829	4.716239	3.390492
26	H	5.069776	6.099588	5.001226	3.925392	2.619841
27	H	5.850544	6.752480	6.144240	5.315691	3.954017
		16	17	18	19	20
16	H	0.000000				
17	H	4.744666	0.000000			
18	H	2.434662	2.473159	0.000000		
19	H	5.573062	4.291426	4.978070	0.000000	
20	H	5.912519	2.500988	4.303800	2.433933	0.000000
21	H	4.742552	9.191604	7.130865	8.089873	9.559257
22	H	5.911268	9.559727	7.975035	7.301758	9.261558
23	H	5.573838	8.092661	7.050955	5.119504	7.304260
24	C	5.448962	6.271987	5.988371	2.600579	4.953306
25	H	5.952223	6.590992	6.426900	2.810358	5.143895
26	H	5.941155	7.232222	6.773165	3.609597	5.964570
27	H	5.931393	6.013131	6.103204	2.028856	4.402781
		21	22	23	24	25
21	H	0.000000				
22	H	2.501136	0.000000			
23	H	4.290453	2.432014	0.000000		
24	C	6.283707	4.968690	2.619163	0.000000	
25	H	6.680114	5.258414	2.926698	1.098822	0.000000
26	H	5.996425	4.371526	1.985255	1.091289	1.764955
27	H	7.207951	5.942091	3.596207	1.092109	1.764960
		26	27			
26	H	0.000000				
27	H	1.750987	0.000000			

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.658996	-0.996033	0.020090
2	6	0	-2.460918	-1.660387	-0.008318
3	6	0	-1.218336	-0.949567	-0.018815
4	6	0	-1.226224	0.497835	-0.011997
5	6	0	-2.507017	1.145788	0.025575
6	6	0	-3.677900	0.428117	0.041493
7	6	0	0.001802	-1.632237	-0.030686
8	6	0	-0.000525	1.212348	-0.031384
9	6	0	1.227060	0.500838	-0.011882
10	6	0	1.220546	-0.947281	-0.019219
11	6	0	2.463653	-1.657420	-0.009246
12	1	0	2.434600	-2.744801	-0.020308
13	6	0	3.661383	-0.992863	0.019469
14	6	0	3.679394	0.431294	0.041943
15	6	0	2.508386	1.148521	0.026469
16	1	0	0.002874	-2.720586	-0.039186
17	1	0	-4.594473	-1.549453	0.029408
18	1	0	-2.431551	-2.747771	-0.018753
19	1	0	-2.558455	2.228168	0.052686
20	1	0	-4.630207	0.950890	0.073544
21	1	0	4.597130	-1.545829	0.028351
22	1	0	4.631351	0.954641	0.074827
23	1	0	2.561048	2.230630	0.055044
24	6	0	-0.008371	2.728359	-0.046778
25	1	0	-0.064752	3.145367	0.968276
26	1	0	0.888706	3.134700	-0.516941
27	1	0	-0.859892	3.120166	-0.607224

```
 Rotational constants (GHZ):      1.3923721      0.4477288
0.3395796
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.7105590342 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
       Virtual  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860557097     A.U. after   11 cycles
             Convg  =    0.5191D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
```

```
 ---------------------------------------------------------------------
      1        6          -0.000145935   -0.000301629   -0.000038801
      2        6           0.000035138    0.000339062   -0.000007799
      3        6          -0.000113663   -0.000053550    0.000002863
      4        6           0.000348117    0.000657534   -0.000007551
      5        6           0.000539408   -0.000414809   -0.000121333
      6        6           0.000330139    0.000380645    0.000080337
      7        6          -0.000108282    0.000228423    0.000067966
      8        6           0.000120227    0.000052423    0.000386159
      9        6          -0.000853177    0.000078851   -0.000034527
     10        6           0.000060652    0.000018255    0.000012990
     11        6          -0.000286621    0.000132139   -0.000017754
     12        1          -0.000014418   -0.000076442   -0.000038730
     13        6           0.000357994   -0.000032790   -0.000043084
     14        6          -0.000547524   -0.000094530    0.000089102
     15        6           0.000172817   -0.000736629   -0.000122704
     16        1           0.000053048   -0.000074964   -0.000009872
     17        1          -0.000086338    0.000053882    0.000034810
     18        1           0.000067556   -0.000026697   -0.000042703
     19        1          -0.000181280    0.000055550    0.000104402
     20        1          -0.000206086   -0.000019515   -0.000008252
     21        1          -0.000006067    0.000098196    0.000037960
     22        1           0.000115266    0.000173159   -0.000017395
     23        1           0.000091664    0.000189742    0.000098472
     24        6           0.000841826   -0.001317935   -0.000027813
     25        1          -0.000037841   -0.000004781    0.000386130
     26        1          -0.000203277    0.000398314   -0.000316048
     27        1          -0.000343340    0.000298097   -0.000446825
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.001317935 RMS     0.000297803


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000806850 RMS     0.000174981
 Search for a local minimum.
 Step number  13 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   13   12
 DE=  8.25D-06 DEPred=-1.19D-06 R=-6.96D+00
 Trust test=-6.96D+00 RLast= 1.02D-01 DXMaxT set to 6.31D-02
 Use linear search instead of GDIIS.
 Quartic linear search produced a step of -0.93597.
 Iteration  1 RMS(Cart)=  0.01188224 RMS(Int)=  0.00018892
 Iteration  2 RMS(Cart)=  0.00019719 RMS(Int)=  0.00000008
```

This journal is © The Royal Society of Chemistry 2014

```
 Iteration  3 RMS(Cart)=  0.00000005 RMS(Int)=  0.00000007
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.58938   0.00011   0.00012   0.00000   0.00012
2.58951
    R2        2.69180  -0.00002   0.00018   0.00000   0.00018
2.69197
    R3        2.05405   0.00000  -0.00009   0.00000  -0.00009
2.05396
    R4        2.70527  -0.00010  -0.00015   0.00000  -0.00015
2.70512
    R5        2.05570   0.00006   0.00016   0.00000   0.00016
2.05587
    R6        2.73527  -0.00021   0.00026   0.00000   0.00026
2.73553
    R7        2.64218  -0.00016  -0.00024   0.00000  -0.00024
2.64194
    R8        2.71338  -0.00035  -0.00063   0.00000  -0.00063
2.71275
    R9        2.68131  -0.00081  -0.00179   0.00000  -0.00179
2.67952
   R10        2.59538  -0.00027  -0.00064   0.00000  -0.00064
2.59474
   R11        2.04835   0.00015   0.00034   0.00000   0.00034
2.04870
   R12        2.05382   0.00021   0.00053   0.00000   0.00053
2.05435
   R13        2.64199  -0.00017  -0.00010   0.00000  -0.00010
2.64189
   R14        2.05675   0.00009   0.00024   0.00000   0.00024
2.05699
   R15        2.68154  -0.00080  -0.00199   0.00000  -0.00199
2.67955
   R16        2.86503  -0.00066  -0.00246   0.00000  -0.00246
2.86257
   R17        2.73661  -0.00011  -0.00070   0.00000  -0.00070
2.73591
   R18        2.71409  -0.00034  -0.00116   0.00000  -0.00116
2.71292
   R19        2.70549  -0.00007  -0.00030   0.00000  -0.00030
2.70519
   R20        2.05569   0.00006   0.00017   0.00000   0.00017
2.05586
   R21        2.58901   0.00009   0.00040   0.00000   0.00040
2.58941
   R22        2.69182  -0.00002   0.00016   0.00000   0.00016
2.69198
   R23        2.05405  -0.00001  -0.00009   0.00000  -0.00009
2.05396
   R24        2.59513  -0.00031  -0.00047   0.00000  -0.00047
2.59466
```

R25	2.05381	0.00021	0.00054	0.00000	0.00054
2.05435					
R26	2.04802	0.00013	0.00059	0.00000	0.00059
2.04861					
R27	2.07647	0.00036	0.00116	0.00000	0.00116
2.07763					
R28	2.06224	0.00032	0.00185	0.00000	0.00185
2.06409					
R29	2.06379	0.00050	0.00077	0.00000	0.00077
2.06455					
A1	2.09054	-0.00025	-0.00124	0.00000	-0.00124
2.08931					
A2	2.10113	0.00023	0.00131	0.00000	0.00131
2.10244					
A3	2.09150	0.00002	-0.00007	0.00000	-0.00007
2.09143					
A4	2.11570	0.00005	0.00061	0.00000	0.00061
2.11631					
A5	2.10418	0.00002	0.00012	0.00000	0.00012
2.10430					
A6	2.06329	-0.00007	-0.00073	0.00000	-0.00073
2.06256					
A7	2.08490	0.00006	0.00039	0.00000	0.00039
2.08529					
A8	2.11190	0.00009	-0.00028	0.00000	-0.00028
2.11162					
A9	2.08637	-0.00015	-0.00011	0.00000	-0.00011
2.08626					
A10	2.04456	-0.00012	-0.00121	0.00000	-0.00121
2.04335					
A11	2.09300	0.00022	0.00013	0.00000	0.00013
2.09313					
A12	2.14560	-0.00011	0.00107	0.00000	0.00107
2.14667					
A13	2.12347	0.00021	0.00103	0.00000	0.00103
2.12450					
A14	2.08702	0.00002	0.00083	0.00000	0.00083
2.08785					
A15	2.07264	-0.00023	-0.00190	0.00000	-0.00190
2.07074					
A16	2.10709	0.00005	0.00037	0.00000	0.00037
2.10746					
A17	2.08631	-0.00004	-0.00020	0.00000	-0.00020
2.08611					
A18	2.08979	-0.00001	-0.00017	0.00000	-0.00017
2.08962					
A19	2.11934	-0.00011	-0.00026	0.00000	-0.00026
2.11907					
A20	2.08193	0.00007	0.00012	0.00000	0.00012
2.08205					
A21	2.08187	0.00005	0.00014	0.00000	0.00014
2.08201					

This journal is © The Royal Society of Chemistry 2014

A22	2.08820	0.00000	-0.00037	0.00000	-0.00037
2.08783					
A23	2.09348	-0.00023	0.00301	0.00000	0.00301
2.09649					
A24	2.10133	0.00023	-0.00259	0.00000	-0.00259
2.09874					
A25	2.09144	0.00012	0.00124	0.00000	0.00124
2.09268					
A26	2.14843	0.00007	-0.00096	0.00000	-0.00096
2.14747					
A27	2.04328	-0.00019	-0.00028	0.00000	-0.00028
2.04300					
A28	2.08734	-0.00009	-0.00079	0.00000	-0.00079
2.08655					
A29	2.11058	0.00001	0.00066	0.00000	0.00066
2.11124					
A30	2.08526	0.00008	0.00013	0.00000	0.00013
2.08539					
A31	2.06298	-0.00008	-0.00051	0.00000	-0.00051
2.06247					
A32	2.11604	0.00006	0.00037	0.00000	0.00037
2.11640					
A33	2.10415	0.00002	0.00014	0.00000	0.00014
2.10429					
A34	2.09018	-0.00027	-0.00098	0.00000	-0.00098
2.08920					
A35	2.10136	0.00024	0.00114	0.00000	0.00114
2.10250					
A36	2.09164	0.00003	-0.00016	0.00000	-0.00016
2.09148					
A37	2.10738	0.00007	0.00016	0.00000	0.00016
2.10755					
A38	2.08632	-0.00005	-0.00021	0.00000	-0.00021
2.08611					
A39	2.08948	-0.00003	0.00005	0.00000	0.00005
2.08953					
A40	2.12412	0.00024	0.00057	0.00000	0.00057
2.12468					
A41	2.08785	0.00005	0.00023	0.00000	0.00023
2.08809					
A42	2.07116	-0.00030	-0.00084	0.00000	-0.00084
2.07032					
A43	1.95020	-0.00028	-0.00017	0.00000	-0.00017
1.95003					
A44	1.95244	0.00045	0.00016	0.00000	0.00016
1.95260					
A45	1.94764	0.00031	0.00358	0.00000	0.00358
1.95122					
A46	1.87429	-0.00002	-0.00023	0.00000	-0.00023
1.87407					
A47	1.87329	0.00002	0.00053	0.00000	0.00053
1.87382					

A48	1.86112	-0.00051	-0.00416	0.00000	-0.00416	1.85696
D1	-0.00146	0.00001	0.00010	0.00000	0.00010	-0.00136
D2	3.13504	0.00000	-0.00024	0.00000	-0.00024	3.13480
D3	-3.13982	0.00003	0.00127	0.00000	0.00127	-3.13855
D4	-0.00332	0.00002	0.00094	0.00000	0.00094	-0.00238
D5	0.00713	0.00003	0.00199	0.00000	0.00199	0.00912
D6	-3.13150	0.00001	0.00157	0.00000	0.00157	-3.12993
D7	-3.13768	0.00001	0.00082	0.00000	0.00082	-3.13685
D8	0.00688	-0.00001	0.00041	0.00000	0.00041	0.00729
D9	-0.01025	-0.00004	-0.00241	0.00000	-0.00241	-0.01266
D10	3.12729	-0.00003	-0.00229	0.00000	-0.00229	3.12500
D11	3.13632	-0.00003	-0.00209	0.00000	-0.00209	3.13423
D12	-0.00932	-0.00002	-0.00197	0.00000	-0.00197	-0.01129
D13	0.01591	0.00003	0.00261	0.00000	0.00261	0.01852
D14	-3.13420	0.00003	0.00190	0.00000	0.00190	-3.13230
D15	-3.12169	0.00002	0.00249	0.00000	0.00249	-3.11920
D16	0.01139	0.00002	0.00178	0.00000	0.00178	0.01316
D17	-3.12334	0.00001	0.00120	0.00000	0.00120	-3.12213
D18	0.00765	0.00000	0.00111	0.00000	0.00111	0.00876
D19	0.01420	0.00001	0.00133	0.00000	0.00133	0.01553
D20	-3.13800	0.00001	0.00124	0.00000	0.00124	-3.13676
D21	-0.01065	0.00001	-0.00061	0.00000	-0.00061	-0.01125
D22	3.11955	-0.00006	-0.00405	0.00000	-0.00405	3.11550
D23	3.13974	0.00001	0.00013	0.00000	0.00013	3.13988
D24	-0.01324	-0.00005	-0.00331	0.00000	-0.00331	-0.01655
D25	-0.03689	-0.00005	-0.00449	0.00000	-0.00449	-0.04138

This journal is © The Royal Society of Chemistry 2014

D26	3.12445	-0.00011	-0.00750	0.00000	-0.00750	3.11695
D27	3.09567	-0.00006	-0.00526	0.00000	-0.00526	3.09041
D28	-0.02618	-0.00012	-0.00827	0.00000	-0.00827	-0.03445
D29	-0.00077	-0.00004	-0.00170	0.00000	-0.00170	-0.00248
D30	3.13784	-0.00002	-0.00128	0.00000	-0.00128	3.13656
D31	-3.13107	0.00002	0.00169	0.00000	0.00169	-3.12938
D32	0.00755	0.00004	0.00211	0.00000	0.00211	0.00966
D33	-0.01380	-0.00001	-0.00165	0.00000	-0.00165	-0.01545
D34	3.12342	-0.00001	-0.00126	0.00000	-0.00126	3.12216
D35	3.13841	-0.00001	-0.00156	0.00000	-0.00156	3.13685
D36	-0.00756	0.00000	-0.00117	0.00000	-0.00117	-0.00873
D37	0.03727	0.00005	0.00419	0.00000	0.00419	0.04146
D38	-3.09513	0.00005	0.00480	0.00000	0.00480	-3.09033
D39	-3.12416	0.00011	0.00726	0.00000	0.00727	-3.11690
D40	0.02663	0.00011	0.00788	0.00000	0.00788	0.03451
D41	1.50773	0.00000	0.04025	0.00000	0.04025	1.54798
D42	-2.67331	0.00009	0.03996	0.00000	0.03996	-2.63336
D43	-0.58979	-0.00004	0.03721	0.00000	0.03721	-0.55258
D44	-1.61397	-0.00006	0.03720	0.00000	0.03720	-1.57677
D45	0.48818	0.00003	0.03690	0.00000	0.03690	0.52508
D46	2.57170	-0.00010	0.03415	0.00000	0.03415	2.60585
D47	-0.01219	-0.00002	-0.00113	0.00000	-0.00113	-0.01333
D48	3.13371	-0.00003	-0.00152	0.00000	-0.00152	3.13219
D49	3.12075	-0.00002	-0.00171	0.00000	-0.00171	3.11903
D50	-0.01654	-0.00003	-0.00210	0.00000	-0.00210	-0.01864
D51	-3.13934	-0.00001	-0.00043	0.00000	-0.00043	-3.13977

```
   D52        0.01415   0.00005   0.00260   0.00000   0.00260
0.01676
   D53        0.01121  -0.00001   0.00016   0.00000   0.00016
0.01137
   D54       -3.11848   0.00005   0.00319   0.00000   0.00319  -
3.11529
   D55        0.00989   0.00002   0.00147   0.00000   0.00147
0.01136
   D56       -3.12669   0.00003   0.00178   0.00000   0.00178  -
3.12491
   D57       -3.13608   0.00003   0.00186   0.00000   0.00186  -
3.13421
   D58        0.01053   0.00004   0.00217   0.00000   0.00217
0.01271
   D59        0.00162  -0.00001  -0.00023   0.00000  -0.00023
0.00139
   D60        3.13985  -0.00003  -0.00130   0.00000  -0.00130
3.13855
   D61       -3.13483   0.00000   0.00009   0.00000   0.00009  -
3.13475
   D62        0.00339  -0.00002  -0.00098   0.00000  -0.00098
0.00241
   D63       -0.00737  -0.00003  -0.00178   0.00000  -0.00178  -
0.00915
   D64        3.13088   0.00000  -0.00104   0.00000  -0.00104
3.12983
   D65        3.13757   0.00000  -0.00072   0.00000  -0.00072
3.13685
   D66       -0.00737   0.00002   0.00001   0.00000   0.00001  -
0.00736
   D67        0.00063   0.00003   0.00180   0.00000   0.00180
0.00243
   D68        3.13044  -0.00002  -0.00120   0.00000  -0.00120
3.12924
   D69       -3.13761   0.00001   0.00106   0.00000   0.00106  -
3.13655
   D70       -0.00781  -0.00004  -0.00193   0.00000  -0.00193  -
0.00974
         Item               Value     Threshold  Converged?
 Maximum Force            0.000807     0.000450     NO
 RMS     Force            0.000175     0.000300     YES
 Maximum Displacement     0.084855     0.001800     NO
 RMS     Displacement     0.011890     0.001200     NO
 Predicted change in Energy=-9.569817D-09

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

1	6	0	-4.791994	-5.432398	0.005818
2	6	0	-3.422398	-5.398215	-0.022162
3	6	0	-2.710494	-4.156352	-0.033318
4	6	0	-3.449455	-2.911596	-0.030684
5	6	0	-4.881634	-3.002035	0.006934
6	6	0	-5.528359	-4.213117	0.025973
7	6	0	-1.312752	-4.128005	-0.042003
8	6	0	-2.754100	-1.676067	-0.053081
9	6	0	-1.336400	-1.669095	-0.026950
10	6	0	-0.608325	-2.920482	-0.029708
11	6	0	0.823013	-2.902887	-0.014911
12	1	0	1.348499	-3.855430	-0.024384
13	6	0	1.519353	-1.723179	0.016730
14	6	0	0.812426	-0.486597	0.037137
15	6	0	-0.560207	-0.462121	0.014674
16	1	0	-0.761065	-5.066330	-0.048539
17	1	0	-5.319344	-6.382740	0.016850
18	1	0	-2.846012	-6.320851	-0.031448
19	1	0	-5.475313	-2.095345	0.034856
20	1	0	-6.614535	-4.243726	0.059187
21	1	0	2.606172	-1.724984	0.030498
22	1	0	1.367613	0.447358	0.073349
23	1	0	-1.062986	0.497896	0.043053
24	6	0	-3.523208	-0.371370	-0.082712
25	1	0	-3.753998	-0.011846	0.930322
26	1	0	-2.965013	0.418679	-0.589949
27	1	0	-4.470915	-0.471178	-0.617014

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370308	0.000000			
3	C	2.441817	1.431487	0.000000		
4	C	2.856254	2.486781	1.447581	0.000000	
5	C	2.432015	2.805689	2.459251	1.435525	0.000000
6	C	1.424530	2.416991	2.819061	2.453367	1.373075
7	C	3.716027	2.462607	1.398056	2.458715	3.742609
8	C	4.273933	3.781794	2.480747	1.417939	2.507627
9	C	5.109271	4.272908	2.841588	2.451289	3.787685
10	C	4.879966	3.749430	2.438545	2.841144	4.274244
11	C	6.158503	4.924452	3.749291	4.272506	5.705550
12	H	6.339826	5.014144	4.070141	4.889910	6.288387
13	C	7.320623	6.158596	4.880004	5.109172	6.527496
14	C	7.474721	6.485464	5.087537	4.903962	6.225003
15	C	6.527768	5.706008	4.274738	3.788105	5.012580
16	H	4.047882	2.682077	2.151410	3.445379	4.609065
17	H	1.086909	2.137572	3.430076	3.943043	3.408938
18	H	2.139530	1.087918	2.168738	3.462249	3.893555
19	H	3.406419	3.889301	3.449149	2.185100	1.084123
20	H	2.176567	3.395468	3.906115	3.435168	2.132481
21	H	8.275167	7.059678	5.846585	6.171094	7.595963

22	H	8.515683	7.558046	6.151137	5.873461	7.138334
23	H	7.005375	6.351001	4.937828	4.162368	5.180048
24	C	5.218396	5.028220	3.871568	2.541829	2.962053
25	H	5.595938	5.479978	4.381146	3.069988	3.326475
26	H	6.158563	5.862409	4.615791	3.411479	3.966231
27	H	5.010460	5.072369	4.125566	2.709760	2.638794
		6	7	8	9	10
6	C	0.000000				
7	C	4.217015	0.000000			
8	C	3.760237	2.844224	0.000000		
9	C	4.903811	2.459070	1.417958	0.000000	
10	C	5.087312	1.398028	2.480618	1.447781	0.000000
11	C	6.485238	2.462345	3.781836	2.487058	1.431523
12	H	6.886338	2.675231	4.645618	3.462478	2.168713
13	C	7.474632	3.715838	4.274283	2.856600	2.441865
14	C	7.354770	4.216930	3.760730	2.453541	2.819007
15	C	6.225162	3.742759	2.508271	1.435617	2.459232
16	H	4.843617	1.088510	3.932695	3.445676	2.151360
17	H	2.179687	4.597834	5.360797	6.171240	5.846632
18	H	3.411866	2.675738	4.645744	4.890581	4.070597
19	H	2.118455	4.632983	2.754728	4.161263	4.936861
20	H	1.087114	5.304012	4.637719	5.873232	6.150889
21	H	8.506552	4.597579	5.361147	3.943387	3.430136
22	H	8.323263	5.303924	4.638258	3.435276	3.906059
23	H	6.491032	4.633420	2.755944	2.185294	3.449249
24	C	4.334912	4.358909	1.514807	2.543488	3.872638
25	H	4.649396	4.883428	2.176352	3.083443	4.390567
26	H	5.329506	4.868526	2.172711	2.707055	4.125269
27	H	3.941284	4.865903	2.171918	3.407104	4.611249
		11	12	13	14	15
11	C	0.000000				
12	H	1.087917	0.000000			
13	C	1.370256	2.139480	0.000000		
14	C	2.416874	3.411774	1.424535	0.000000	
15	C	2.805622	3.893486	2.432045	1.373035	0.000000
16	H	2.681589	2.432513	4.047372	4.843260	4.609022
17	H	7.059670	7.130857	8.275221	8.506675	7.596258
18	H	5.014429	4.865415	6.340136	6.886755	6.289019
19	H	6.350080	7.047398	7.004584	6.490281	5.179392
20	H	7.557808	7.972933	8.515580	8.323236	7.138446
21	H	2.137562	2.474582	1.086907	2.179718	3.408963
22	H	3.395368	4.303941	2.176572	1.087114	2.132389
23	H	3.889175	4.977073	3.406221	2.118119	1.084078
24	C	5.030191	5.989625	5.221562	4.338821	2.965990
25	H	5.495509	6.459108	5.618856	4.677114	3.352829
26	H	5.070761	6.098710	5.006512	3.934693	2.631439
27	H	5.856740	6.757954	6.152434	5.323705	3.961407
		16	17	18	19	20
16	H	0.000000				
17	H	4.745010	0.000000			
18	H	2.433335	2.474578	0.000000		
19	H	5.572957	4.290269	4.977201	0.000000	

20	H	5.911970	2.500938	4.304002	2.431864	0.000000
21	H	4.744378	9.192861	7.131069	8.089969	9.558573
22	H	5.911589	9.558705	7.973348	7.300169	9.258573
23	H	5.573164	8.090762	7.048408	5.117969	7.300887
24	C	5.447316	6.274758	5.988118	2.607034	4.956973
25	H	5.955134	6.623672	6.446161	2.847060	5.181733
26	H	5.935978	7.222907	6.763679	3.607257	5.956375
27	H	5.933091	6.005679	6.099334	2.017837	4.391409

		21	22	23	24	25
21	H	0.000000				
22	H	2.500987	0.000000			
23	H	4.289997	2.431313	0.000000		
24	C	6.278088	4.961331	2.612305	0.000000	
25	H	6.648029	5.213077	2.878998	1.099436	0.000000
26	H	6.001529	4.383200	2.006160	1.092267	1.766090
27	H	7.216402	5.950523	3.603994	1.092514	1.766127

		26	27
26	H	0.000000	
27	H	1.749376	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.659973	-0.994596	0.021684
2	6	0	-2.461841	-1.658793	-0.010971
3	6	0	-1.218961	-0.948649	-0.020937
4	6	0	-1.225522	0.498889	-0.012047
5	6	0	-2.506097	1.146243	0.030297
6	6	0	-3.677175	0.429587	0.048011
7	6	0	0.000511	-1.632219	-0.034413
8	6	0	-0.000137	1.212004	-0.033216
9	6	0	1.225767	0.499745	-0.012008
10	6	0	1.219584	-0.947995	-0.021004
11	6	0	2.462611	-1.657956	-0.011147
12	1	0	2.433132	-2.745381	-0.025267
13	6	0	3.660650	-0.993701	0.021554
14	6	0	3.677594	0.430486	0.048081
15	6	0	2.506483	1.147014	0.030477
16	1	0	0.000830	-2.720671	-0.045646
17	1	0	-4.596055	-1.546883	0.031746
18	1	0	-2.432283	-2.746219	-0.024993
19	1	0	-2.558615	2.228600	0.062970
20	1	0	-4.629126	0.953272	0.084922
21	1	0	4.596806	-1.545861	0.031526
22	1	0	4.629447	0.954338	0.085118

```
    23          1          0        2.559354    2.229300    0.063447
    24          6          0       -0.002375    2.726634   -0.056307
    25          1          0       -0.017706    3.149150    0.958584
    26          1          0        0.878351    3.127233   -0.563150
    27          1          0       -0.870849    3.122961   -0.587594
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3930275      0.4478968
0.3397405
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8699715203 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860565392     A.U. after   11 cycles
             Convg  =    0.4864D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000000581   -0.000021471   -0.000003890
      2        6          -0.000013101    0.000035007    0.000000785
      3        6          -0.000032887    0.000001346    0.000004937
      4        6           0.000034210    0.000030786    0.000005153
      5        6           0.000051300   -0.000028024   -0.000010778
      6        6           0.000029249    0.000024086    0.000006482
      7        6          -0.000003300    0.000018647   -0.000001324
      8        6           0.000006719    0.000042446    0.000015158
      9        6          -0.000070269   -0.000005415   -0.000006787
     10        6           0.000008301    0.000013714    0.000005186
     11        6          -0.000018262    0.000030999    0.000000463
     12        1          -0.000003335   -0.000017293   -0.000001878
     13        6           0.000021755   -0.000017043   -0.000004770
     14        6          -0.000044240   -0.000011183    0.000006985
     15        6           0.000015419   -0.000065951   -0.000010969
     16        1           0.000007919   -0.000011764    0.000004660
     17        1          -0.000011772    0.000000816    0.000003371
     18        1           0.000015520   -0.000006001   -0.000001675
     19        1          -0.000019990    0.000008962    0.000005795
     20        1          -0.000021098    0.000000248   -0.000002397
     21        1           0.000004893    0.000010166    0.000003923
     22        1           0.000009463    0.000018841   -0.000003344
     23        1           0.000010680    0.000022087    0.000006101
```

```
     24        6           0.000101536   -0.000151258    0.000000786
     25        1          -0.000014336    0.000010823    0.000012449
     26        1          -0.000037781    0.000032258   -0.000005939
     27        1          -0.000027174    0.000034173   -0.000028483
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000151258 RMS     0.000029154


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000074589 RMS     0.000016226
 Search for a local minimum.
 Step number  14 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
     Eigenvalues ---   -0.00153   0.00021   0.01539   0.01690
0.01775
     Eigenvalues ---    0.01801   0.01818   0.01825   0.01881
0.01976
     Eigenvalues ---    0.01982   0.02018   0.02057   0.02096
0.02112
     Eigenvalues ---    0.02140   0.02146   0.02191   0.02226
0.02268
     Eigenvalues ---    0.02346   0.02468   0.06092   0.06685
0.06833
     Eigenvalues ---    0.13023   0.15529   0.15969   0.15999
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16005   0.16060
0.16190
     Eigenvalues ---    0.16582   0.19675   0.21647   0.21999
0.22608
     Eigenvalues ---    0.23308   0.23959   0.24411   0.24776
0.25012
     Eigenvalues ---    0.26359   0.28673   0.31769   0.33587
0.33630
     Eigenvalues ---    0.33634   0.33682   0.33682   0.33748
0.33998
     Eigenvalues ---    0.34014   0.34375   0.36964   0.37269
0.37530
     Eigenvalues ---    0.37899   0.38528   0.39473   0.39845
0.40436
     Eigenvalues ---    0.41129   0.41688   0.45094   0.45333
0.46124
```

```
     Eigenvalues ---    0.49225   0.49769   0.49835   0.51309
0.55961
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is  -1.53D-03 should be greater than     0.000000
Eigenvector:
                          D41       D42       D43       D28       D44
   1                    0.31526   0.30816   0.30743  -0.25109
0.23739
                          D45       D46       D26       D39       D40
   1                    0.23028   0.22955  -0.20733   0.20104
0.17907
 Use linear search instead of GDIIS.
 RFO step:  Lambda=-6.07892943D-07 EMin= 1.53439372D-03
 Quartic linear search produced a step of -0.00028.
 Iteration  1 RMS(Cart)=  0.00235046 RMS(Int)=  0.00000751
 Iteration  2 RMS(Cart)=  0.00000783 RMS(Int)=  0.00000004
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000004
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58951   0.00000   0.00000   0.00049   0.00049
2.58999
    R2        2.69197   0.00000   0.00000  -0.00030  -0.00030
2.69167
```

This journal is © The Royal Society of Chemistry 2014

R3	2.05396	0.00001	0.00000	-0.00012	-0.00012
2.05384					
R4	2.70512	-0.00001	0.00000	-0.00025	-0.00025
2.70487					
R5	2.05587	0.00001	0.00000	-0.00015	-0.00015
2.05572					
R6	2.73553	-0.00003	0.00000	0.00016	0.00016
2.73569					
R7	2.64194	0.00000	0.00000	-0.00017	-0.00017
2.64177					
R8	2.71275	-0.00003	0.00000	-0.00067	-0.00067
2.71208					
R9	2.67952	-0.00005	0.00000	-0.00067	-0.00067
2.67884					
R10	2.59474	-0.00002	0.00000	0.00011	0.00011
2.59484					
R11	2.04870	0.00002	0.00000	0.00010	0.00010
2.04879					
R12	2.05435	0.00002	0.00000	0.00004	0.00004
2.05439					
R13	2.64189	-0.00001	0.00000	-0.00012	-0.00012
2.64177					
R14	2.05699	0.00001	0.00000	-0.00009	-0.00009
2.05690					
R15	2.67955	-0.00006	0.00000	-0.00024	-0.00024
2.67931					
R16	2.86257	-0.00007	0.00000	-0.00090	-0.00090
2.86167					
R17	2.73591	-0.00001	0.00000	0.00032	0.00032
2.73623					
R18	2.71292	-0.00002	0.00000	-0.00046	-0.00046
2.71247					
R19	2.70519	-0.00001	0.00000	-0.00025	-0.00025
2.70494					
R20	2.05586	0.00001	0.00000	-0.00015	-0.00015
2.05572					
R21	2.58941	0.00000	0.00000	0.00043	0.00043
2.58984					
R22	2.69198	0.00000	0.00000	-0.00038	-0.00038
2.69160					
R23	2.05396	0.00000	0.00000	-0.00012	-0.00012
2.05384					
R24	2.59466	-0.00002	0.00000	0.00011	0.00011
2.59477					
R25	2.05435	0.00002	0.00000	0.00004	0.00004
2.05439					
R26	2.04861	0.00001	0.00000	-0.00007	-0.00007
2.04854					
R27	2.07763	0.00002	0.00000	0.00065	0.00065
2.07828					
R28	2.06409	0.00001	0.00000	0.00063	0.00063
2.06472					

This journal is © The Royal Society of Chemistry 2014

R29	2.06455	0.00003	0.00000	0.00077	0.00077
2.06532					
A1	2.08931	-0.00002	0.00000	-0.00012	-0.00012
2.08918					
A2	2.10244	0.00002	0.00000	-0.00021	-0.00021
2.10223					
A3	2.09143	0.00000	0.00000	0.00034	0.00034
2.09177					
A4	2.11631	0.00001	0.00000	0.00015	0.00015
2.11646					
A5	2.10430	0.00001	0.00000	-0.00034	-0.00034
2.10396					
A6	2.06256	-0.00001	0.00000	0.00019	0.00019
2.06275					
A7	2.08529	0.00001	0.00000	-0.00028	-0.00028
2.08501					
A8	2.11162	0.00000	0.00000	0.00047	0.00047
2.11209					
A9	2.08626	-0.00002	0.00000	-0.00019	-0.00019
2.08608					
A10	2.04335	-0.00001	0.00000	0.00019	0.00019
2.04354					
A11	2.09313	0.00003	0.00000	0.00034	0.00034
2.09347					
A12	2.14667	-0.00001	0.00000	-0.00053	-0.00053
2.14614					
A13	2.12450	0.00001	0.00000	0.00016	0.00016
2.12466					
A14	2.08785	0.00001	0.00000	0.00016	0.00016
2.08801					
A15	2.07074	-0.00002	0.00000	-0.00032	-0.00032
2.07043					
A16	2.10746	0.00000	0.00000	-0.00009	-0.00009
2.10737					
A17	2.08611	0.00000	0.00000	0.00043	0.00043
2.08654					
A18	2.08962	0.00000	0.00000	-0.00034	-0.00034
2.08928					
A19	2.11907	-0.00001	0.00000	0.00001	0.00001
2.11908					
A20	2.08205	0.00001	0.00000	-0.00001	-0.00001
2.08204					
A21	2.08201	0.00000	0.00000	0.00000	0.00000
2.08201					
A22	2.08783	0.00000	0.00000	-0.00011	-0.00011
2.08772					
A23	2.09649	-0.00004	0.00000	-0.00061	-0.00061
2.09588					
A24	2.09874	0.00004	0.00000	0.00072	0.00072
2.09946					
A25	2.09268	0.00001	0.00000	0.00005	0.00005
2.09273					

A26	2.14747	0.00002	0.00000	0.00005	0.00005	2.14752
A27	2.04300	-0.00002	0.00000	-0.00011	-0.00011	2.04289
A28	2.08655	-0.00001	0.00000	-0.00007	-0.00007	2.08648
A29	2.11124	-0.00001	0.00000	0.00022	0.00022	2.11146
A30	2.08539	0.00001	0.00000	-0.00015	-0.00015	2.08524
A31	2.06247	-0.00002	0.00000	0.00018	0.00018	2.06266
A32	2.11640	0.00001	0.00000	0.00020	0.00020	2.11660
A33	2.10429	0.00001	0.00000	-0.00038	-0.00038	2.10392
A34	2.08920	-0.00003	0.00000	-0.00018	-0.00018	2.08902
A35	2.10250	0.00002	0.00000	-0.00019	-0.00019	2.10231
A36	2.09148	0.00000	0.00000	0.00036	0.00036	2.09184
A37	2.10755	0.00001	0.00000	-0.00005	-0.00005	2.10749
A38	2.08611	0.00000	0.00000	0.00038	0.00038	2.08649
A39	2.08953	-0.00001	0.00000	-0.00033	-0.00033	2.08920
A40	2.12468	0.00002	0.00000	0.00029	0.00029	2.12497
A41	2.08809	0.00001	0.00000	0.00038	0.00038	2.08846
A42	2.07032	-0.00003	0.00000	-0.00067	-0.00067	2.06965
A43	1.95003	0.00000	0.00000	0.00012	0.00012	1.95015
A44	1.95260	0.00006	0.00000	0.00082	0.00082	1.95342
A45	1.95122	0.00003	0.00000	0.00022	0.00022	1.95144
A46	1.87407	-0.00002	0.00000	-0.00015	-0.00015	1.87392
A47	1.87382	-0.00002	0.00000	-0.00047	-0.00047	1.87335
A48	1.85696	-0.00005	0.00000	-0.00064	-0.00064	1.85632
D1	-0.00136	0.00000	0.00000	-0.00007	-0.00007	-0.00144
D2	3.13480	0.00000	0.00000	0.00022	0.00022	3.13502
D3	-3.13855	0.00000	0.00000	-0.00015	-0.00015	-3.13870

This journal is © The Royal Society of Chemistry 2014

D4	-0.00238	0.00000	0.00000	0.00014	0.00014	-0.00224
D5	0.00912	0.00000	0.00000	-0.00029	-0.00029	0.00883
D6	-3.12993	0.00000	0.00000	-0.00037	-0.00037	-3.13029
D7	-3.13685	0.00000	0.00000	-0.00022	-0.00022	-3.13707
D8	0.00729	0.00000	0.00000	-0.00029	-0.00029	0.00700
D9	-0.01266	0.00000	0.00000	0.00034	0.00034	-0.01232
D10	3.12500	0.00000	0.00000	0.00034	0.00034	3.12535
D11	3.13423	0.00000	0.00000	0.00006	0.00006	3.13429
D12	-0.01129	0.00000	0.00000	0.00006	0.00006	-0.01123
D13	0.01852	0.00000	0.00000	-0.00024	-0.00024	0.01828
D14	-3.13230	0.00000	0.00000	-0.00006	-0.00006	-3.13236
D15	-3.11920	0.00000	0.00000	-0.00024	-0.00024	-3.11944
D16	0.01316	0.00000	0.00000	-0.00007	-0.00007	0.01310
D17	-3.12213	0.00000	0.00000	-0.00072	-0.00072	-3.12285
D18	0.00876	0.00000	0.00000	-0.00086	-0.00086	0.00790
D19	0.01553	0.00000	0.00000	-0.00071	-0.00072	0.01481
D20	-3.13676	0.00000	0.00000	-0.00085	-0.00086	-3.13762
D21	-0.01125	0.00000	0.00000	-0.00012	-0.00012	-0.01138
D22	3.11550	0.00000	0.00000	0.00003	0.00003	3.11554
D23	3.13988	0.00000	0.00000	-0.00031	-0.00031	3.13957
D24	-0.01655	0.00000	0.00000	-0.00015	-0.00015	-0.01670
D25	-0.04138	0.00000	0.00000	0.00076	0.00076	-0.04063
D26	3.11695	0.00000	0.00000	0.00108	0.00108	3.11803
D27	3.09041	0.00000	0.00000	0.00094	0.00095	3.09136
D28	-0.03445	0.00000	0.00000	0.00127	0.00127	-0.03317
D29	-0.00248	0.00000	0.00000	0.00039	0.00039	-0.00209

D30	3.13656	0.00000	0.00000	0.00047	0.00047	3.13703
D31	-3.12938	0.00000	0.00000	0.00023	0.00023	-3.12915
D32	0.00966	0.00000	0.00000	0.00031	0.00031	0.00997
D33	-0.01545	0.00000	0.00000	0.00080	0.00080	-0.01465
D34	3.12216	0.00000	0.00000	0.00063	0.00063	3.12279
D35	3.13685	0.00000	0.00000	0.00094	0.00094	3.13778
D36	-0.00873	0.00000	0.00000	0.00077	0.00077	-0.00796
D37	0.04146	0.00000	0.00000	-0.00068	-0.00068	0.04077
D38	-3.09033	0.00000	0.00000	-0.00053	-0.00053	-3.09086
D39	-3.11690	0.00000	0.00000	-0.00102	-0.00102	-3.11791
D40	0.03451	0.00000	0.00000	-0.00087	-0.00087	0.03364
D41	1.54798	-0.00001	-0.00001	-0.00798	-0.00799	1.53999
D42	-2.63336	0.00000	-0.00001	-0.00752	-0.00753	-2.64089
D43	-0.55258	0.00000	-0.00001	-0.00762	-0.00763	-0.56021
D44	-1.57677	-0.00001	-0.00001	-0.00765	-0.00766	-1.58443
D45	0.52508	0.00000	-0.00001	-0.00719	-0.00720	0.51788
D46	2.60585	-0.00001	-0.00001	-0.00729	-0.00730	2.59856
D47	-0.01333	0.00000	0.00000	-0.00009	-0.00009	-0.01342
D48	3.13219	0.00000	0.00000	0.00007	0.00007	3.13226
D49	3.11903	0.00000	0.00000	-0.00023	-0.00023	3.11880
D50	-0.01864	0.00000	0.00000	-0.00007	-0.00007	-0.01871
D51	-3.13977	0.00000	0.00000	0.00024	0.00024	-3.13953
D52	0.01676	0.00000	0.00000	0.00023	0.00023	0.01698
D53	0.01137	0.00000	0.00000	0.00038	0.00038	0.01176
D54	-3.11529	0.00000	0.00000	0.00037	0.00037	-3.11492
D55	0.01136	0.00000	0.00000	0.00023	0.00023	0.01159

```
   D56       -3.12491   0.00000   0.00000   0.00000   0.00000  -
3.12491
   D57       -3.13421   0.00000   0.00000   0.00007   0.00007  -
3.13414
   D58        0.01271   0.00000   0.00000  -0.00017  -0.00017
0.01254
   D59        0.00139   0.00000   0.00000   0.00010   0.00010
0.00149
   D60        3.13855   0.00000   0.00000   0.00002   0.00002
3.13857
   D61       -3.13475   0.00000   0.00000  -0.00014  -0.00014  -
3.13489
   D62        0.00241   0.00000   0.00000  -0.00023  -0.00022
0.00219
   D63       -0.00915   0.00000   0.00000   0.00021   0.00021  -
0.00894
   D64        3.12983   0.00000   0.00000   0.00027   0.00028
3.13011
   D65        3.13685   0.00000   0.00000   0.00030   0.00030
3.13714
   D66       -0.00736   0.00000   0.00000   0.00036   0.00036  -
0.00700
   D67        0.00243   0.00000   0.00000  -0.00046  -0.00046
0.00197
   D68        3.12924   0.00000   0.00000  -0.00044  -0.00044
3.12880
   D69       -3.13655   0.00000   0.00000  -0.00053  -0.00053  -
3.13707
   D70       -0.00974   0.00000   0.00000  -0.00051  -0.00051  -
0.01024
         Item               Value     Threshold  Converged?
 Maximum Force            0.000075     0.000450     YES
 RMS     Force            0.000016     0.000300     YES
 Maximum Displacement     0.014845     0.001800     NO
 RMS     Displacement     0.002351     0.001200     NO
 Predicted change in Energy=-6.835650D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792370   -5.431772    0.005787
      2          6           0       -3.422491   -5.398014   -0.021423
      3          6           0       -2.710074   -4.156596   -0.032624
      4          6           0       -3.448854   -2.911630   -0.030438
      5          6           0       -4.880729   -3.001517    0.006480
      6          6           0       -5.528136   -4.212304    0.025162
      7          6           0       -1.312420   -4.128246   -0.040931
```

8	6	0	-2.753866	-1.676302	-0.052793
9	6	0	-1.336285	-1.669283	-0.027123
10	6	0	-0.608030	-2.920763	-0.029533
11	6	0	0.823178	-2.902837	-0.015114
12	1	0	1.349015	-3.855100	-0.024374
13	6	0	1.519608	-1.722894	0.015651
14	6	0	0.812531	-0.486619	0.035623
15	6	0	-0.560179	-0.462519	0.013865
16	1	0	-0.760753	-5.066536	-0.046319
17	1	0	-5.319790	-6.382007	0.016715
18	1	0	-2.846742	-6.320963	-0.030306
19	1	0	-5.474261	-2.094656	0.034015
20	1	0	-6.614388	-4.241968	0.057414
21	1	0	2.606369	-1.724864	0.029116
22	1	0	1.367199	0.447708	0.070875
23	1	0	-1.062546	0.497668	0.042326
24	6	0	-3.523733	-0.372583	-0.081450
25	1	0	-3.761324	-0.017546	0.931968
26	1	0	-2.963800	0.420895	-0.582094
27	1	0	-4.468555	-0.470766	-0.621960

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370565	0.000000			
3	C	2.442029	1.431357	0.000000		
4	C	2.856127	2.486540	1.447667	0.000000	
5	C	2.431861	2.805430	2.459163	1.435169	0.000000
6	C	1.424370	2.416986	2.819205	2.453214	1.373132
7	C	3.716371	2.462741	1.397966	2.458579	3.742271
8	C	4.273463	3.781426	2.480762	1.417583	2.506642
9	C	5.109004	4.272671	2.841487	2.450792	3.786695
10	C	4.880073	3.749403	2.438417	2.840838	4.273614
11	C	6.158760	4.924597	3.749145	4.272068	5.704801
12	H	6.340616	5.014764	4.070278	4.889756	6.288025
13	C	7.320993	6.158914	4.880107	5.108897	6.526812
14	C	7.474647	6.485404	5.087448	4.903513	6.224048
15	C	6.527249	5.705540	4.274390	3.787420	5.011359
16	H	4.048463	2.682414	2.151286	3.445251	4.608828
17	H	1.086848	2.137625	3.430089	3.942860	3.408899
18	H	2.139493	1.087841	2.168679	3.462093	3.893222
19	H	3.406187	3.889088	3.449169	2.184920	1.084174
20	H	2.176706	3.395713	3.906285	3.434840	2.132343
21	H	8.275449	7.059868	5.846511	6.170712	7.595195
22	H	8.515445	7.557917	6.150973	5.872800	7.137079
23	H	7.005083	6.350786	4.937828	4.162100	5.179199
24	C	5.216554	5.026809	3.870811	2.540663	2.959808
25	H	5.588802	5.474779	4.378047	3.065875	3.318686
26	H	6.159787	5.863826	4.617327	3.412524	3.966603
27	H	5.011038	5.072739	4.126126	2.710629	2.639986

		6	7	8	9	10
6	C	0.000000				

7	C	4.217072	0.000000			
8	C	3.759516	2.844281	0.000000		
9	C	4.903193	2.459117	1.417830	0.000000	
10	C	5.087093	1.397966	2.480692	1.447951	0.000000
11	C	6.485023	2.462330	3.781673	2.486982	1.431393
12	H	6.886600	2.675466	4.645599	3.462461	2.168649
13	C	7.474487	3.716087	4.274276	2.856717	2.442085
14	C	7.354244	4.216956	3.760632	2.453578	2.819095
15	C	6.224277	3.742515	2.507983	1.435375	2.459093
16	H	4.843838	1.088464	3.932712	3.445712	2.151266
17	H	2.179700	4.598019	5.360266	6.170899	5.846625
18	H	3.411656	2.676241	4.645643	4.890768	4.071018
19	H	2.118351	4.632712	2.753744	4.160231	4.936263
20	H	1.087135	5.304099	4.636639	5.872327	6.150567
21	H	8.506324	4.597614	5.361081	3.943447	3.430157
22	H	8.322466	5.303980	4.637875	3.435125	3.906176
23	H	6.490426	4.633406	2.756041	2.185277	3.449264
24	C	4.332719	4.358503	1.514332	2.543484	3.872627
25	H	4.641112	4.882777	2.176281	3.086892	4.392768
26	H	5.330207	4.869763	2.173124	2.706592	4.125730
27	H	3.942155	4.865793	2.171965	3.406082	4.610543

		11	12	13	14	15
11	C	0.000000				
12	H	1.087839	0.000000			
13	C	1.370484	2.139394	0.000000		
14	C	2.416774	3.411462	1.424336	0.000000	
15	C	2.805293	3.893082	2.431884	1.373094	0.000000
16	H	2.681679	2.432936	4.047694	4.843302	4.608776
17	H	7.059865	7.131613	8.275548	8.506546	7.595673
18	H	5.015189	4.866712	6.341085	6.887248	6.289013
19	H	6.349276	7.046961	7.003767	6.489186	5.178077
20	H	7.557507	7.973214	8.515243	8.322394	7.137197
21	H	2.137603	2.474208	1.086846	2.179713	3.408925
22	H	3.395512	4.303900	2.176647	1.087136	2.132263
23	H	3.888791	4.976612	3.405749	2.117730	1.084040
24	C	5.030132	5.989562	5.221883	4.339343	2.966451
25	H	5.499048	6.461963	5.624597	4.684401	3.359798
26	H	5.070489	6.098816	5.005405	3.932662	2.629255
27	H	5.855397	6.756844	6.150811	5.321893	3.959767

		16	17	18	19	20
16	H	0.000000				
17	H	4.745446	0.000000			
18	H	2.434172	2.474248	0.000000		
19	H	5.572762	4.290167	4.976912	0.000000	
20	H	5.912336	2.501481	4.304076	2.431334	0.000000
21	H	4.744467	9.193102	7.131905	8.089088	9.558189
22	H	5.911750	9.558439	7.973859	7.298667	9.257374
23	H	5.573087	8.090409	7.048571	5.116976	7.299817
24	C	5.446878	6.272849	5.986998	2.604501	4.954146
25	H	5.954223	6.616107	6.441700	2.838109	5.172094
26	H	5.937370	7.224177	6.765413	3.606937	5.956345
27	H	5.932981	6.006270	6.099601	2.019596	4.391823

This journal is © The Royal Society of Chemistry 2014

		21	22	23	24	25
21	H	0.000000				
22	H	2.501471	0.000000			
23	H	4.289611	2.430426	0.000000		
24	C	6.278459	4.961582	2.613446	0.000000	
25	H	6.654141	5.221081	2.887960	1.099781	0.000000
26	H	6.000387	4.380028	2.002639	1.092600	1.766538
27	H	7.214653	5.948079	3.602782	1.092922	1.766431

		26	27
26	H	0.000000	
27	H	1.749553	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.659913	-0.994425	0.021207
2	6	0	-2.461631	-1.658926	-0.010554
3	6	0	-1.218657	-0.949206	-0.020394
4	6	0	-1.225211	0.498422	-0.011909
5	6	0	-2.505363	1.145876	0.029600
6	6	0	-3.676758	0.429615	0.046794
7	6	0	0.000862	-1.632516	-0.033362
8	6	0	-0.000366	1.211764	-0.032862
9	6	0	1.225580	0.499822	-0.011986
10	6	0	1.219760	-0.948091	-0.020681
11	6	0	2.462965	-1.657482	-0.011069
12	1	0	2.434124	-2.744849	-0.025014
13	6	0	3.661080	-0.992857	0.020923
14	6	0	3.677486	0.431144	0.047061
15	6	0	2.505996	1.147180	0.030040
16	1	0	0.001376	-2.720933	-0.043482
17	1	0	-4.595906	-1.546748	0.031032
18	1	0	-2.432588	-2.746293	-0.024203
19	1	0	-2.557862	2.228297	0.061912
20	1	0	-4.628392	0.953990	0.082645
21	1	0	4.597197	-1.544966	0.030690
22	1	0	4.628981	0.955750	0.083274
23	1	0	2.559114	2.229412	0.063130
24	6	0	-0.004015	2.725931	-0.054934
25	1	0	-0.027681	3.147987	0.960362
26	1	0	0.879948	3.128748	-0.555059
27	1	0	-0.869191	3.122091	-0.592528

Rotational constants (GHZ): 1.3933363 0.4479416
0.3397808

This journal is © The Royal Society of Chemistry 2014

```
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9186661964 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860564994     A.U. after    9 cycles
            Convg  =    0.7495D-08             -V/T =  2.0100
```

```
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000263175   -0.000023753   -0.000015735
      2        6          -0.000226044   -0.000028089    0.000003655
      3        6          -0.000155939    0.000117640    0.000015553
      4        6           0.000063435   -0.000184556   -0.000005877
      5        6          -0.000215867   -0.000065229    0.000003618
      6        6          -0.000016949    0.000107453    0.000016086
      7        6           0.000044400   -0.000041534   -0.000002117
      8        6           0.000149677    0.000044077    0.000019074
      9        6           0.000009940   -0.000082471    0.000009045
     10        6          -0.000063634    0.000144721    0.000017884
     11        6           0.000148422    0.000187359    0.000000682
     12        1           0.000000698   -0.000078218    0.000005747
     13        6          -0.000088315   -0.000260627   -0.000014594
     14        6          -0.000114681    0.000071052    0.000012646
     15        6           0.000167030    0.000084902   -0.000008970
     16        1           0.000028657   -0.000041349   -0.000024599
     17        1          -0.000043741   -0.000024408    0.000000925
     18        1           0.000061508   -0.000042744    0.000003029
     19        1           0.000019342   -0.000009928   -0.000003510
     20        1          -0.000006256   -0.000040758    0.000009174
     21        1           0.000043057    0.000025447   -0.000003090
     22        1           0.000027814   -0.000010868    0.000011861
     23        1          -0.000031468    0.000017408   -0.000010613
     24        6          -0.000131658    0.000356512   -0.000072264
     25        1           0.000042368   -0.000062422   -0.000174907
     26        1          -0.000141045   -0.000167381    0.000133589
     27        1           0.000166074    0.000007763    0.000073710
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000356512 RMS     0.000100504


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000283437 RMS     0.000058272
 Search for a local minimum.
 Step number  15 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
```

This journal is © The Royal Society of Chemistry 2014

```
                                                     11   12   13   15
14
 DE=  3.98D-07 DEPred=-6.84D-07 R=-5.82D-01
 Trust test=-5.82D-01 RLast= 1.92D-02 DXMaxT set to 5.00D-02
 Use linear search instead of GDIIS.
 Quartic linear search produced a step of -0.69928.
 Iteration  1 RMS(Cart)=  0.00164388 RMS(Int)=  0.00000367
 Iteration  2 RMS(Cart)=  0.00000383 RMS(Int)=  0.00000001
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000001
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.58999  -0.00019  -0.00034   0.00000  -0.00034
2.58965
    R2        2.69167   0.00007   0.00021   0.00000   0.00021
2.69188
    R3        2.05384   0.00004   0.00008   0.00000   0.00008
2.05393
    R4        2.70487   0.00004   0.00017   0.00000   0.00017
2.70504
    R5        2.05572   0.00007   0.00010   0.00000   0.00010
2.05582
    R6        2.73569  -0.00007  -0.00011   0.00000  -0.00011
2.73558
    R7        2.64177   0.00007   0.00012   0.00000   0.00012
2.64189
    R8        2.71208   0.00019   0.00047   0.00000   0.00047
2.71255
    R9        2.67884   0.00028   0.00047   0.00000   0.00047
2.67931
   R10        2.59484  -0.00001  -0.00007   0.00000  -0.00007
2.59477
   R11        2.04879  -0.00002  -0.00007   0.00000  -0.00007
2.04872
   R12        2.05439   0.00001  -0.00003   0.00000  -0.00003
2.05436
   R13        2.64177   0.00005   0.00008   0.00000   0.00008
2.64185
   R14        2.05690   0.00005   0.00006   0.00000   0.00006
2.05696
   R15        2.67931   0.00010   0.00017   0.00000   0.00017
2.67948
   R16        2.86167   0.00015   0.00063   0.00000   0.00063
2.86230
   R17        2.73623  -0.00004  -0.00023   0.00000  -0.00023
2.73601
   R18        2.71247   0.00012   0.00032   0.00000   0.00032
2.71279
   R19        2.70494   0.00005   0.00017   0.00000   0.00017
2.70511
   R20        2.05572   0.00007   0.00010   0.00000   0.00010
2.05582
```

This journal is © The Royal Society of Chemistry 2014

R21	2.58984	-0.00018	-0.00030	0.00000	-0.00030
2.58954					
R22	2.69160	0.00010	0.00026	0.00000	0.00026
2.69187					
R23	2.05384	0.00004	0.00008	0.00000	0.00008
2.05392					
R24	2.59477	-0.00003	-0.00008	0.00000	-0.00008
2.59469					
R25	2.05439	0.00001	-0.00003	0.00000	-0.00003
2.05436					
R26	2.04854	0.00003	0.00005	0.00000	0.00005
2.04859					
R27	2.07828	-0.00019	-0.00046	0.00000	-0.00046
2.07783					
R28	2.06472	-0.00026	-0.00044	0.00000	-0.00044
2.06428					
R29	2.06532	-0.00018	-0.00054	0.00000	-0.00054
2.06478					
A1	2.08918	0.00002	0.00009	0.00000	0.00009
2.08927					
A2	2.10223	0.00002	0.00015	0.00000	0.00015
2.10237					
A3	2.09177	-0.00003	-0.00024	0.00000	-0.00024
2.09153					
A4	2.11646	0.00000	-0.00011	0.00000	-0.00011
2.11636					
A5	2.10396	0.00003	0.00024	0.00000	0.00024
2.10419					
A6	2.06275	-0.00003	-0.00013	0.00000	-0.00013
2.06262					
A7	2.08501	0.00007	0.00020	0.00000	0.00020
2.08521					
A8	2.11209	-0.00009	-0.00033	0.00000	-0.00033
2.11176					
A9	2.08608	0.00001	0.00013	0.00000	0.00013
2.08621					
A10	2.04354	-0.00008	-0.00013	0.00000	-0.00013
2.04341					
A11	2.09347	-0.00004	-0.00024	0.00000	-0.00024
2.09323					
A12	2.14614	0.00011	0.00037	0.00000	0.00037
2.14651					
A13	2.12466	-0.00003	-0.00011	0.00000	-0.00011
2.12455					
A14	2.08801	0.00000	-0.00011	0.00000	-0.00011
2.08790					
A15	2.07043	0.00002	0.00022	0.00000	0.00022
2.07065					
A16	2.10737	0.00001	0.00006	0.00000	0.00006
2.10743					
A17	2.08654	-0.00005	-0.00030	0.00000	-0.00030
2.08623					

This journal is © The Royal Society of Chemistry 2014

A18	2.08928	0.00004	0.00024	0.00000	0.00024
2.08952					
A19	2.11908	0.00002	0.00000	0.00000	0.00000
2.11907					
A20	2.08204	-0.00001	0.00001	0.00000	0.00001
2.08205					
A21	2.08201	-0.00002	0.00000	0.00000	0.00000
2.08201					
A22	2.08772	0.00000	0.00008	0.00000	0.00008
2.08779					
A23	2.09588	-0.00001	0.00043	0.00000	0.00043
2.09631					
A24	2.09946	0.00001	-0.00050	0.00000	-0.00050
2.09896					
A25	2.09273	-0.00003	-0.00004	0.00000	-0.00004
2.09270					
A26	2.14752	0.00009	-0.00004	0.00000	-0.00004
2.14749					
A27	2.04289	-0.00005	0.00007	0.00000	0.00007
2.04296					
A28	2.08648	0.00004	0.00005	0.00000	0.00005
2.08653					
A29	2.11146	-0.00010	-0.00015	0.00000	-0.00015
2.11130					
A30	2.08524	0.00006	0.00011	0.00000	0.00011
2.08535					
A31	2.06266	-0.00004	-0.00013	0.00000	-0.00013
2.06253					
A32	2.11660	0.00000	-0.00014	0.00000	-0.00014
2.11646					
A33	2.10392	0.00004	0.00027	0.00000	0.00027
2.10418					
A34	2.08902	0.00001	0.00012	0.00000	0.00012
2.08915					
A35	2.10231	0.00002	0.00013	0.00000	0.00013
2.10244					
A36	2.09184	-0.00003	-0.00025	0.00000	-0.00025
2.09159					
A37	2.10749	0.00002	0.00004	0.00000	0.00004
2.10753					
A38	2.08649	-0.00004	-0.00027	0.00000	-0.00027
2.08622					
A39	2.08920	0.00002	0.00023	0.00000	0.00023
2.08943					
A40	2.12497	-0.00003	-0.00020	0.00000	-0.00020
2.12477					
A41	2.08846	-0.00001	-0.00026	0.00000	-0.00026
2.08820					
A42	2.06965	0.00003	0.00047	0.00000	0.00047
2.07012					
A43	1.95015	-0.00001	-0.00008	0.00000	-0.00008
1.95006					

A44	1.95342	0.00004	-0.00057	0.00000	-0.00057	1.95285
A45	1.95144	-0.00002	-0.00015	0.00000	-0.00015	1.95128
A46	1.87392	-0.00002	0.00011	0.00000	0.00011	1.87402
A47	1.87335	0.00001	0.00033	0.00000	0.00033	1.87368
A48	1.85632	0.00000	0.00044	0.00000	0.00045	1.85677
D1	-0.00144	0.00000	0.00005	0.00000	0.00005	-0.00138
D2	3.13502	-0.00001	-0.00015	0.00000	-0.00015	3.13487
D3	-3.13870	0.00000	0.00011	0.00000	0.00011	-3.13859
D4	-0.00224	0.00000	-0.00010	0.00000	-0.00010	-0.00234
D5	0.00883	0.00001	0.00020	0.00000	0.00020	0.00903
D6	-3.13029	0.00001	0.00026	0.00000	0.00026	-3.13004
D7	-3.13707	0.00000	0.00015	0.00000	0.00015	-3.13692
D8	0.00700	0.00000	0.00021	0.00000	0.00021	0.00720
D9	-0.01232	-0.00001	-0.00024	0.00000	-0.00024	-0.01256
D10	3.12535	0.00000	-0.00024	0.00000	-0.00024	3.12511
D11	3.13429	0.00000	-0.00004	0.00000	-0.00004	3.13425
D12	-0.01123	0.00000	-0.00004	0.00000	-0.00004	-0.01127
D13	0.01828	0.00000	0.00017	0.00000	0.00017	0.01845
D14	-3.13236	0.00000	0.00004	0.00000	0.00004	-3.13232
D15	-3.11944	0.00000	0.00017	0.00000	0.00017	-3.11927
D16	0.01310	0.00000	0.00005	0.00000	0.00005	0.01314
D17	-3.12285	0.00001	0.00050	0.00000	0.00050	-3.12235
D18	0.00790	0.00001	0.00060	0.00000	0.00060	0.00850
D19	0.01481	0.00001	0.00050	0.00000	0.00050	0.01531
D20	-3.13762	0.00001	0.00060	0.00000	0.00060	-3.13702
D21	-0.01138	0.00000	0.00008	0.00000	0.00008	-0.01129

This journal is © The Royal Society of Chemistry 2014

D22	3.11554	0.00000	-0.00002	0.00000	-0.00002	3.11551
D23	3.13957	0.00001	0.00021	0.00000	0.00021	3.13978
D24	-0.01670	0.00000	0.00011	0.00000	0.00011	-0.01660
D25	-0.04063	-0.00001	-0.00053	0.00000	-0.00053	-0.04116
D26	3.11803	-0.00002	-0.00076	0.00000	-0.00076	3.11727
D27	3.09136	-0.00002	-0.00066	0.00000	-0.00066	3.09070
D28	-0.03317	-0.00002	-0.00089	0.00000	-0.00089	-0.03406
D29	-0.00209	-0.00001	-0.00027	0.00000	-0.00027	-0.00236
D30	3.13703	-0.00001	-0.00033	0.00000	-0.00033	3.13670
D31	-3.12915	0.00000	-0.00016	0.00000	-0.00016	-3.12931
D32	0.00997	0.00000	-0.00022	0.00000	-0.00022	0.00976
D33	-0.01465	-0.00001	-0.00056	0.00000	-0.00056	-0.01521
D34	3.12279	-0.00001	-0.00044	0.00000	-0.00044	3.12235
D35	3.13778	-0.00001	-0.00065	0.00000	-0.00065	3.13713
D36	-0.00796	-0.00001	-0.00054	0.00000	-0.00054	-0.00850
D37	0.04077	0.00001	0.00048	0.00000	0.00048	0.04125
D38	-3.09086	0.00001	0.00037	0.00000	0.00037	-3.09049
D39	-3.11791	0.00002	0.00071	0.00000	0.00071	-3.11720
D40	0.03364	0.00001	0.00061	0.00000	0.00061	0.03424
D41	1.53999	-0.00001	0.00559	0.00000	0.00559	1.54558
D42	-2.64089	-0.00001	0.00527	0.00000	0.00527	-2.63562
D43	-0.56021	-0.00001	0.00534	0.00000	0.00534	-0.55488
D44	-1.58443	-0.00001	0.00536	0.00000	0.00536	-1.57907
D45	0.51788	-0.00001	0.00503	0.00000	0.00503	0.52291
D46	2.59856	-0.00001	0.00510	0.00000	0.00510	2.60366
D47	-0.01342	0.00000	0.00006	0.00000	0.00006	-0.01335

```
   D48        3.13226  -0.00001  -0.00005   0.00000  -0.00005
3.13221
   D49        3.11880   0.00001   0.00016   0.00000   0.00016
3.11896
   D50       -0.01871   0.00000   0.00005   0.00000   0.00005  -
0.01866
   D51       -3.13953   0.00000  -0.00017   0.00000  -0.00017  -
3.13970
   D52        0.01698   0.00000  -0.00016   0.00000  -0.00016
0.01682
   D53        0.01176  -0.00001  -0.00027   0.00000  -0.00027
0.01149
   D54       -3.11492  -0.00001  -0.00026   0.00000  -0.00026  -
3.11518
   D55        0.01159  -0.00001  -0.00016   0.00000  -0.00016
0.01143
   D56       -3.12491   0.00000   0.00000   0.00000   0.00000  -
3.12491
   D57       -3.13414   0.00000  -0.00005   0.00000  -0.00005  -
3.13419
   D58        0.01254   0.00000   0.00012   0.00000   0.00012
0.01266
   D59        0.00149   0.00000  -0.00007   0.00000  -0.00007
0.00142
   D60        3.13857   0.00000  -0.00001   0.00000  -0.00001
3.13856
   D61       -3.13489   0.00000   0.00010   0.00000   0.00010  -
3.13479
   D62        0.00219   0.00000   0.00016   0.00000   0.00016
0.00235
   D63       -0.00894  -0.00001  -0.00015   0.00000  -0.00015  -
0.00909
   D64        3.13011   0.00000  -0.00019   0.00000  -0.00019
3.12992
   D65        3.13714  -0.00001  -0.00021   0.00000  -0.00021
3.13694
   D66       -0.00700   0.00000  -0.00025   0.00000  -0.00025  -
0.00725
   D67        0.00197   0.00001   0.00032   0.00000   0.00032
0.00229
   D68        3.12880   0.00001   0.00031   0.00000   0.00031
3.12911
   D69       -3.13707   0.00001   0.00037   0.00000   0.00037  -
3.13670
   D70       -0.01024   0.00001   0.00035   0.00000   0.00035  -
0.00989
         Item               Value     Threshold  Converged?
 Maximum Force            0.000283     0.000450     YES
 RMS     Force            0.000058     0.000300     YES
 Maximum Displacement     0.010386     0.001800     NO
 RMS     Displacement     0.001644     0.001200     NO
 Predicted change in Energy=-8.827953D-08
```

This journal is © The Royal Society of Chemistry 2014

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.792107	-5.432209	0.005809
2	6	0	-3.422426	-5.398155	-0.021940
3	6	0	-2.710367	-4.156426	-0.033109
4	6	0	-3.449274	-2.911606	-0.030610
5	6	0	-4.881362	-3.001879	0.006797
6	6	0	-5.528292	-4.212872	0.025729
7	6	0	-1.312652	-4.128078	-0.041681
8	6	0	-2.754030	-1.676138	-0.052994
9	6	0	-1.336366	-1.669152	-0.027002
10	6	0	-0.608236	-2.920566	-0.029655
11	6	0	0.823063	-2.902872	-0.014972
12	1	0	1.348654	-3.855331	-0.024381
13	6	0	1.519430	-1.723094	0.016406
14	6	0	0.812458	-0.486603	0.036681
15	6	0	-0.560198	-0.462240	0.014431
16	1	0	-0.760971	-5.066392	-0.047872
17	1	0	-5.319478	-6.382520	0.016809
18	1	0	-2.846231	-6.320885	-0.031104
19	1	0	-5.474997	-2.095138	0.034603
20	1	0	-6.614491	-4.243197	0.058654
21	1	0	2.606231	-1.724948	0.030082
22	1	0	1.367489	0.447463	0.072605
23	1	0	-1.062853	0.497828	0.042834
24	6	0	-3.523366	-0.371735	-0.082333
25	1	0	-3.756202	-0.013559	0.930823
26	1	0	-2.964644	0.419348	-0.587590
27	1	0	-4.470209	-0.471058	-0.618504

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370386	0.000000			
3	C	2.441881	1.431448	0.000000		
4	C	2.856216	2.486709	1.447607	0.000000	
5	C	2.431969	2.805611	2.459225	1.435418	0.000000
6	C	1.424482	2.416990	2.819105	2.453321	1.373092
7	C	3.716130	2.462647	1.398029	2.458674	3.742508
8	C	4.273791	3.781683	2.480752	1.417832	2.507331
9	C	5.109191	4.272837	2.841558	2.451140	3.787387
10	C	4.879999	3.749422	2.438507	2.841052	4.274054
11	C	6.158581	4.924496	3.749247	4.272374	5.705325
12	H	6.340063	5.014331	4.070183	4.889864	6.288278
13	C	7.320735	6.158692	4.880035	5.109089	6.527290

14	C	7.474699	6.485446	5.087510	4.903827	6.224716
15	C	6.527612	5.705867	4.274634	3.787899	5.012213
16	H	4.048057	2.682178	2.151372	3.445341	4.608993
17	H	1.086890	2.137588	3.430080	3.942988	3.408926
18	H	2.139519	1.087895	2.168720	3.462202	3.893455
19	H	3.406349	3.889237	3.449155	2.185046	1.084138
20	H	2.176609	3.395541	3.906166	3.435070	2.132439
21	H	8.275252	7.059735	5.846563	6.170979	7.595732
22	H	8.515612	7.558007	6.151088	5.873262	7.137957
23	H	7.005287	6.350936	4.937828	4.162287	5.179793
24	C	5.217842	5.027796	3.871340	2.541478	2.961378
25	H	5.593794	5.478416	4.380215	3.068752	3.324134
26	H	6.158934	5.862837	4.616255	3.411795	3.966346
27	H	5.010629	5.072476	4.125732	2.710019	2.639148

		6	7	8	9	10
6	C	0.000000				
7	C	4.217032	0.000000			
8	C	3.760020	2.844241	0.000000		
9	C	4.903626	2.459084	1.417919	0.000000	
10	C	5.087246	1.398009	2.480640	1.447832	0.000000
11	C	6.485173	2.462340	3.781787	2.487035	1.431484
12	H	6.886417	2.675301	4.645612	3.462473	2.168694
13	C	7.474589	3.715913	4.274281	2.856635	2.441931
14	C	7.354612	4.216938	3.760700	2.453552	2.819033
15	C	6.224896	3.742686	2.508184	1.435544	2.459190
16	H	4.843683	1.088496	3.932700	3.445687	2.151332
17	H	2.179691	4.597890	5.360637	6.171138	5.846630
18	H	3.411803	2.675889	4.645714	4.890637	4.070724
19	H	2.118424	4.632902	2.754432	4.160953	4.936681
20	H	1.087121	5.304038	4.637394	5.872960	6.150792
21	H	8.506484	4.597589	5.361127	3.943405	3.430142
22	H	8.323024	5.303941	4.638143	3.435231	3.906094
23	H	6.490850	4.633416	2.755973	2.185289	3.449253
24	C	4.334252	4.358787	1.514664	2.543487	3.872635
25	H	4.646906	4.883233	2.176331	3.084481	4.391230
26	H	5.329720	4.868899	2.172835	2.706914	4.125406
27	H	3.941541	4.865869	2.171932	3.406798	4.611037

		11	12	13	14	15
11	C	0.000000				
12	H	1.087893	0.000000			
13	C	1.370324	2.139454	0.000000		
14	C	2.416844	3.411680	1.424475	0.000000	
15	C	2.805523	3.893364	2.431997	1.373052	0.000000
16	H	2.681616	2.432640	4.047469	4.843273	4.608948
17	H	7.059729	7.131084	8.275320	8.506637	7.596082
18	H	5.014658	4.865805	6.340421	6.886904	6.289017
19	H	6.349839	7.047267	7.004338	6.489952	5.178997
20	H	7.557718	7.973018	8.515479	8.322983	7.138071
21	H	2.137575	2.474470	1.086889	2.179717	3.408952
22	H	3.395411	4.303929	2.176594	1.087120	2.132351
23	H	3.889059	4.976934	3.406080	2.118002	1.084066
24	C	5.030173	5.989606	5.221658	4.338978	2.966129

This journal is © The Royal Society of Chemistry 2014

25	H	5.496574	6.459967	5.620584	4.679307	3.354926
26	H	5.070677	6.098740	5.006175	3.934077	2.630777
27	H	5.856338	6.757622	6.151949	5.323164	3.960918

		16	17	18	19	20
16	H	0.000000				
17	H	4.745141	0.000000			
18	H	2.433587	2.474479	0.000000		
19	H	5.572898	4.290239	4.977114	0.000000	
20	H	5.912080	2.501102	4.304024	2.431704	0.000000
21	H	4.744405	9.192933	7.131320	8.089704	9.558458
22	H	5.911638	9.558625	7.973502	7.299718	9.258212
23	H	5.573141	8.090656	7.048457	5.117670	7.300565
24	C	5.447185	6.274184	5.987781	2.606272	4.956123
25	H	5.954862	6.621399	6.444821	2.844370	5.178836
26	H	5.936398	7.223292	6.764203	3.607164	5.956370
27	H	5.933057	6.005852	6.099411	2.018361	4.391529

		21	22	23	24	25
21	H	0.000000				
22	H	2.501132	0.000000			
23	H	4.289881	2.431046	0.000000		
24	C	6.278200	4.961407	2.612648	0.000000	
25	H	6.649868	5.215485	2.881695	1.099540	0.000000
26	H	6.001182	4.382240	2.005094	1.092367	1.766225
27	H	7.215879	5.949792	3.603634	1.092637	1.766218

		26	27
26	H	0.000000	
27	H	1.749429	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.659955	-0.994545	0.021541
2	6	0	-2.461778	-1.658833	-0.010845
3	6	0	-1.218870	-0.948817	-0.020774
4	6	0	-1.225429	0.498749	-0.012005
5	6	0	-2.505876	1.146133	0.030088
6	6	0	-3.677050	0.429596	0.047645
7	6	0	0.000617	-1.632309	-0.034097
8	6	0	-0.000206	1.211932	-0.033109
9	6	0	1.225711	0.499768	-0.012001
10	6	0	1.219637	-0.948024	-0.020907
11	6	0	2.462718	-1.657813	-0.011123
12	1	0	2.433431	-2.745221	-0.025191
13	6	0	3.660779	-0.993447	0.021364
14	6	0	3.677562	0.430684	0.047774

```
     15          6           0        2.506337    1.147064    0.030346
     16          1           0        0.000994   -2.720750   -0.044995
     17          1           0       -4.596010   -1.546842    0.031531
     18          1           0       -2.432375   -2.746242   -0.024755
     19          1           0       -2.558388    2.228509    0.062651
     20          1           0       -4.628905    0.953488    0.084238
     21          1           0        4.596923   -1.545592    0.031275
     22          1           0        4.629307    0.954763    0.084563
     23          1           0        2.559282    2.229334    0.063352
     24          6           0       -0.002868    2.726423   -0.055894
     25          1           0       -0.020705    3.148803    0.959125
     26          1           0        0.878837    3.127689   -0.560720
     27          1           0       -0.870356    3.122698   -0.589080
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3931203      0.4479102
0.3397526
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8846063452 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860565483     A.U. after    9 cycles
            Convg  =    0.5231D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000079584   -0.000022127   -0.000007480
      2        6          -0.000077170    0.000016024    0.000001667
      3        6          -0.000069901    0.000036284    0.000008157
      4        6           0.000042951   -0.000033906    0.000001853
      5        6          -0.000029010   -0.000039234   -0.000006420
      6        6           0.000015366    0.000049151    0.000009379
      7        6           0.000011033    0.000000541   -0.000001569
      8        6           0.000049595    0.000042922    0.000016190
      9        6          -0.000046119   -0.000028539   -0.000002032
     10        6          -0.000013327    0.000053113    0.000009024
     11        6           0.000031877    0.000078021    0.000000552
     12        1          -0.000002125   -0.000035622    0.000000409
     13        6          -0.000011361   -0.000090267   -0.000007753
     14        6          -0.000065424    0.000013524    0.000008693
     15        6           0.000061024   -0.000020609   -0.000010328
     16        1           0.000014155   -0.000020654   -0.000004144
     17        1          -0.000021384   -0.000006767    0.000002639
     18        1           0.000029355   -0.000017042   -0.000000266
     19        1          -0.000008166    0.000003260    0.000003014
     20        1          -0.000016623   -0.000012081    0.000001076
     21        1           0.000016366    0.000014759    0.000001818
     22        1           0.000014977    0.000009901    0.000001223
     23        1          -0.000001969    0.000020675    0.000001104
     24        6           0.000031443    0.000001426   -0.000021334
     25        1           0.000002451   -0.000011396   -0.000043885
     26        1          -0.000068812   -0.000027687    0.000036337
     27        1           0.000031215    0.000026330    0.000002075
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000090267 RMS     0.000031389
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000072599 RMS     0.000017717
 Search for a local minimum.
 Step number  16 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16
     Eigenvalues ---   -0.58630   0.00002   0.01220   0.01632
0.01771
     Eigenvalues ---    0.01790   0.01819   0.01822   0.01863
0.01942
     Eigenvalues ---    0.01976   0.01982   0.02040   0.02070
0.02101
     Eigenvalues ---    0.02116   0.02144   0.02154   0.02201
0.02227
     Eigenvalues ---    0.02316   0.02348   0.03818   0.06606
0.06856
     Eigenvalues ---    0.12311   0.14829   0.15694   0.15999
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16006   0.16021
0.16179
     Eigenvalues ---    0.16211   0.19808   0.21985   0.22050
0.22310
     Eigenvalues ---    0.22621   0.23443   0.24449   0.24712
0.24985
     Eigenvalues ---    0.26781   0.28398   0.32843   0.33508
0.33620
     Eigenvalues ---    0.33631   0.33667   0.33682   0.33684
0.33751
     Eigenvalues ---    0.34048   0.34153   0.36759   0.36823
0.37239
     Eigenvalues ---    0.37509   0.38455   0.39386   0.39700
0.40454
     Eigenvalues ---    0.41122   0.41619   0.44303   0.45359
0.48216
     Eigenvalues ---    0.49364   0.49833   0.50201   0.51307
0.56173
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is  -5.86D-01 should be greater than     0.000000
Eigenvector:
                          A44       R6        R28       A48       A24
   1                    0.30836  -0.24672  -0.20355  -0.19351
0.18425
                          R21       R9        R15       A35       A29
   1                   -0.17568   0.16892  -0.16886   0.16235  -
0.16167
 Eigenvalue     2 is   2.40D-05 Eigenvector:
                          D44       D45       D46       D41       D42
   1                    0.43251   0.41629   0.41624   0.39686
0.38064
                          D43       D27       D38       D15       A23
   1                    0.38059  -0.05830   0.03811   0.03387
0.02967
 Use linear search instead of GDIIS.
 RFO step:  Lambda=-1.34793021D-06 EMin= 5.86303015D-01
 Quartic linear search produced a step of -0.00311.
 Maximum step size (   0.050) exceeded in Quadratic search.
    -- Step size scaled by   0.465
 Iteration  1 RMS(Cart)=  0.00577864 RMS(Int)=  0.00005240
 Iteration  2 RMS(Cart)=  0.00005435 RMS(Int)=  0.00000030
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000030
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
```

This journal is © The Royal Society of Chemistry 2014

			(Linear)	(Quad)	(Total)	
R1	2.58965	-0.00005	0.00000	0.00025	0.00025	2.58990
R2	2.69188	0.00002	0.00000	-0.00019	-0.00019	2.69169
R3	2.05393	0.00002	0.00000	-0.00001	-0.00001	2.05392
R4	2.70504	0.00000	0.00000	-0.00017	-0.00017	2.70487
R5	2.05582	0.00003	0.00000	-0.00003	-0.00003	2.05579
R6	2.73558	-0.00004	0.00000	0.00003	0.00003	2.73561
R7	2.64189	0.00002	0.00000	-0.00007	-0.00007	2.64183
R8	2.71255	0.00004	0.00000	-0.00027	-0.00027	2.71228
R9	2.67931	0.00005	0.00000	-0.00014	-0.00014	2.67917
R10	2.59477	-0.00001	0.00000	0.00017	0.00017	2.59494
R11	2.04872	0.00001	0.00000	0.00005	0.00005	2.04877
R12	2.05436	0.00002	0.00000	-0.00004	-0.00004	2.05432
R13	2.64185	0.00001	0.00000	-0.00004	-0.00004	2.64182
R14	2.05696	0.00002	0.00000	-0.00002	-0.00002	2.05694
R15	2.67948	-0.00001	0.00000	0.00034	0.00034	2.67982
R16	2.86230	-0.00001	0.00000	0.00052	0.00051	2.86281
R17	2.73601	-0.00002	0.00000	0.00047	0.00047	2.73648
R18	2.71279	0.00002	0.00000	0.00007	0.00007	2.71286
R19	2.70511	0.00001	0.00000	-0.00013	-0.00013	2.70498
R20	2.05582	0.00003	0.00000	-0.00003	-0.00003	2.05579
R21	2.58954	-0.00006	0.00000	0.00012	0.00012	2.58966
R22	2.69187	0.00003	0.00000	-0.00027	-0.00027	2.69160
R23	2.05392	0.00002	0.00000	-0.00001	-0.00001	2.05391
R24	2.59469	-0.00003	0.00000	0.00012	0.00013	2.59482
R25	2.05436	0.00002	0.00000	-0.00004	-0.00004	2.05432

This journal is © The Royal Society of Chemistry 2014

R26	2.04859	0.00002	0.00000	-0.00018	-0.00018
2.04840					
R27	2.07783	-0.00004	0.00000	-0.00005	-0.00004
2.07778					
R28	2.06428	-0.00007	0.00000	-0.00022	-0.00021
2.06406					
R29	2.06478	-0.00003	0.00000	0.00027	0.00027
2.06506					
A1	2.08927	-0.00001	0.00000	0.00025	0.00025
2.08952					
A2	2.10237	0.00002	0.00000	-0.00048	-0.00048
2.10189					
A3	2.09153	-0.00001	0.00000	0.00024	0.00024
2.09177					
A4	2.11636	0.00000	0.00000	-0.00002	-0.00002
2.11634					
A5	2.10419	0.00001	0.00000	-0.00040	-0.00040
2.10379					
A6	2.06262	-0.00002	0.00000	0.00042	0.00042
2.06304					
A7	2.08521	0.00003	0.00000	-0.00033	-0.00033
2.08488					
A8	2.11176	-0.00002	0.00000	0.00049	0.00049
2.11226					
A9	2.08621	-0.00001	0.00000	-0.00016	-0.00016
2.08605					
A10	2.04341	-0.00003	0.00000	0.00045	0.00045
2.04386					
A11	2.09323	0.00001	0.00000	0.00025	0.00025
2.09348					
A12	2.14651	0.00002	0.00000	-0.00069	-0.00069
2.14582					
A13	2.12455	0.00000	0.00000	-0.00012	-0.00012
2.12442					
A14	2.08790	0.00000	0.00000	-0.00028	-0.00028
2.08762					
A15	2.07065	-0.00001	0.00000	0.00040	0.00040
2.07105					
A16	2.10743	0.00001	0.00000	-0.00021	-0.00021
2.10722					
A17	2.08623	-0.00001	0.00000	0.00023	0.00023
2.08646					
A18	2.08952	0.00001	0.00000	-0.00001	-0.00001
2.08950					
A19	2.11907	0.00000	0.00000	0.00009	0.00009
2.11917					
A20	2.08205	0.00000	0.00000	-0.00004	-0.00004
2.08201					
A21	2.08201	0.00000	0.00000	-0.00005	-0.00005
2.08197					
A22	2.08779	0.00000	0.00000	0.00009	0.00009
2.08789					

This journal is © The Royal Society of Chemistry 2014

A23	2.09631	-0.00003	0.00000	-0.00152	-0.00153
2.09478					
A24	2.09896	0.00003	0.00000	0.00146	0.00146
2.10042					
A25	2.09270	0.00000	0.00000	-0.00038	-0.00038
2.09231					
A26	2.14749	0.00004	0.00000	0.00050	0.00050
2.14799					
A27	2.04296	-0.00003	0.00000	-0.00011	-0.00011
2.04285					
A28	2.08653	0.00001	0.00000	0.00017	0.00017
2.08670					
A29	2.11130	-0.00003	0.00000	-0.00005	-0.00005
2.11125					
A30	2.08535	0.00003	0.00000	-0.00012	-0.00012
2.08522					
A31	2.06253	-0.00002	0.00000	0.00036	0.00036
2.06289					
A32	2.11646	0.00000	0.00000	0.00009	0.00009
2.11656					
A33	2.10418	0.00002	0.00000	-0.00045	-0.00046
2.10373					
A34	2.08915	-0.00002	0.00000	0.00012	0.00012
2.08926					
A35	2.10244	0.00002	0.00000	-0.00042	-0.00042
2.10203					
A36	2.09159	-0.00001	0.00000	0.00030	0.00030
2.09188					
A37	2.10753	0.00001	0.00000	-0.00011	-0.00011
2.10742					
A38	2.08622	-0.00001	0.00000	0.00017	0.00017
2.08639					
A39	2.08943	0.00000	0.00000	-0.00006	-0.00006
2.08937					
A40	2.12477	0.00001	0.00000	0.00014	0.00014
2.12491					
A41	2.08820	0.00000	0.00000	0.00013	0.00013
2.08833					
A42	2.07012	-0.00001	0.00000	-0.00028	-0.00028
2.06984					
A43	1.95006	0.00000	0.00000	0.00008	0.00008
1.95015					
A44	1.95285	0.00005	0.00000	0.00038	0.00038
1.95324					
A45	1.95128	0.00002	0.00000	-0.00111	-0.00111
1.95017					
A46	1.87402	-0.00002	0.00000	0.00039	0.00039
1.87441					
A47	1.87368	-0.00001	0.00000	-0.00007	-0.00007
1.87360					
A48	1.85677	-0.00004	0.00000	0.00038	0.00038
1.85714					

This journal is © The Royal Society of Chemistry 2014

D1	-0.00138	0.00000	0.00000	0.00036	0.00036	-0.00102
D2	3.13487	0.00000	0.00000	0.00037	0.00037	3.13524
D3	-3.13859	0.00000	0.00000	-0.00006	-0.00006	-3.13865
D4	-0.00234	0.00000	0.00000	-0.00004	-0.00004	-0.00238
D5	0.00903	0.00000	0.00000	-0.00026	-0.00026	0.00877
D6	-3.13004	0.00000	0.00000	-0.00059	-0.00059	-3.13063
D7	-3.13692	0.00000	0.00000	0.00015	0.00015	-3.13677
D8	0.00720	0.00000	0.00000	-0.00018	-0.00018	0.00702
D9	-0.01256	0.00000	0.00000	0.00038	0.00038	-0.01218
D10	3.12511	0.00000	0.00000	0.00106	0.00106	3.12617
D11	3.13425	0.00000	0.00000	0.00037	0.00037	3.13462
D12	-0.01127	0.00000	0.00000	0.00105	0.00105	-0.01022
D13	0.01845	0.00000	0.00000	-0.00117	-0.00117	0.01728
D14	-3.13232	0.00000	0.00000	0.00030	0.00030	-3.13202
D15	-3.11927	0.00000	0.00000	-0.00184	-0.00184	-3.12111
D16	0.01314	0.00000	0.00000	-0.00037	-0.00037	0.01277
D17	-3.12235	0.00000	0.00000	-0.00159	-0.00159	-3.12394
D18	0.00850	0.00000	0.00000	-0.00075	-0.00076	0.00774
D19	0.01531	0.00000	0.00000	-0.00092	-0.00092	0.01440
D20	-3.13702	0.00000	0.00000	-0.00008	-0.00008	-3.13710
D21	-0.01129	0.00000	0.00000	0.00129	0.00129	-0.01000
D22	3.11551	0.00000	0.00000	0.00111	0.00111	3.11663
D23	3.13978	0.00000	0.00000	-0.00023	-0.00023	3.13955
D24	-0.01660	0.00000	0.00000	-0.00041	-0.00041	-0.01701
D25	-0.04116	0.00000	0.00000	0.00155	0.00155	-0.03961
D26	3.11727	-0.00001	0.00000	-0.00047	-0.00047	3.11681

This journal is © The Royal Society of Chemistry 2014

D27	3.09070	-0.00001	0.00000	0.00312	0.00312	3.09381
D28	-0.03406	-0.00001	0.00000	0.00110	0.00110	-0.03296
D29	-0.00236	0.00000	0.00000	-0.00060	-0.00060	-0.00296
D30	3.13670	0.00000	0.00000	-0.00027	-0.00027	3.13643
D31	-3.12931	0.00000	0.00000	-0.00041	-0.00041	-3.12972
D32	0.00976	0.00000	0.00000	-0.00008	-0.00008	0.00967
D33	-0.01521	0.00000	0.00000	0.00099	0.00100	-0.01421
D34	3.12235	0.00000	0.00000	0.00142	0.00143	3.12378
D35	3.13713	0.00000	0.00000	0.00016	0.00016	3.13728
D36	-0.00850	0.00000	0.00000	0.00058	0.00059	-0.00791
D37	0.04125	0.00000	0.00000	-0.00148	-0.00148	0.03977
D38	-3.09049	0.00000	0.00000	-0.00207	-0.00207	-3.09256
D39	-3.11720	0.00001	0.00000	0.00051	0.00051	-3.11669
D40	0.03424	0.00000	0.00000	-0.00008	-0.00008	0.03417
D41	1.54558	-0.00001	-0.00002	-0.01970	-0.01972	1.52586
D42	-2.63562	0.00000	-0.00002	-0.01888	-0.01890	-2.65452
D43	-0.55488	-0.00001	-0.00002	-0.01889	-0.01891	-0.57379
D44	-1.57907	-0.00001	-0.00002	-0.02172	-0.02174	-1.60081
D45	0.52291	0.00000	-0.00002	-0.02090	-0.02091	0.50200
D46	2.60366	-0.00001	-0.00002	-0.02091	-0.02093	2.58273
D47	-0.01335	0.00000	0.00000	0.00022	0.00022	-0.01313
D48	3.13221	0.00000	0.00000	-0.00020	-0.00020	3.13201
D49	3.11896	0.00000	0.00000	0.00078	0.00078	3.11974
D50	-0.01866	0.00000	0.00000	0.00035	0.00035	-0.01830
D51	-3.13970	0.00000	0.00000	-0.00004	-0.00004	-3.13974
D52	0.01682	0.00000	0.00000	0.00051	0.00051	0.01734

```
   D53        0.01149   0.00000   0.00000  -0.00061  -0.00061
0.01088
   D54       -3.11518   0.00000   0.00000  -0.00006  -0.00006  -
3.11523
   D55        0.01143   0.00000   0.00000  -0.00048  -0.00048
0.01095
   D56       -3.12491   0.00000   0.00000  -0.00038  -0.00038  -
3.12529
   D57       -3.13419   0.00000   0.00000  -0.00005  -0.00005  -
3.13424
   D58        0.01266   0.00000   0.00000   0.00005   0.00005
0.01271
   D59        0.00142   0.00000   0.00000  -0.00021  -0.00021
0.00121
   D60        3.13856   0.00000   0.00000  -0.00017  -0.00017
3.13839
   D61       -3.13479   0.00000   0.00000  -0.00012  -0.00012  -
3.13490
   D62        0.00235   0.00000   0.00000  -0.00007  -0.00007
0.00228
   D63       -0.00909   0.00000   0.00000  -0.00004  -0.00004  -
0.00912
   D64        3.12992   0.00000   0.00000   0.00020   0.00020
3.13011
   D65        3.13694   0.00000   0.00000  -0.00008  -0.00008
3.13685
   D66       -0.00725   0.00000   0.00000   0.00015   0.00015  -
0.00710
   D67        0.00229   0.00000   0.00000   0.00046   0.00046
0.00276
   D68        3.12911   0.00000   0.00000  -0.00008  -0.00008
3.12903
   D69       -3.13670   0.00000   0.00000   0.00023   0.00023  -
3.13648
   D70       -0.00989   0.00000   0.00000  -0.00031  -0.00032  -
0.01021
         Item               Value     Threshold  Converged?
 Maximum Force            0.000073     0.000450     YES
 RMS     Force            0.000018     0.000300     YES
 Maximum Displacement     0.038934     0.001800     NO
 RMS     Displacement     0.005778     0.001200     NO
 Predicted change in Energy=-5.903226D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792339   -5.431291    0.006033
```

This journal is © The Royal Society of Chemistry 2014

2	6	0	-3.422488	-5.397838	-0.020524
3	6	0	-2.709935	-4.156491	-0.030968
4	6	0	-3.448728	-2.911582	-0.028518
5	6	0	-4.880780	-3.001090	0.006587
6	6	0	-5.528262	-4.211898	0.024974
7	6	0	-1.312257	-4.128059	-0.039594
8	6	0	-2.753699	-1.676072	-0.050545
9	6	0	-1.335830	-1.668800	-0.026068
10	6	0	-0.607818	-2.920572	-0.028767
11	6	0	0.823430	-2.902969	-0.015881
12	1	0	1.349280	-3.855265	-0.025231
13	6	0	1.520059	-1.723227	0.013871
14	6	0	0.813530	-0.486644	0.033971
15	6	0	-0.559210	-0.462058	0.013116
16	1	0	-0.760561	-5.066354	-0.045673
17	1	0	-5.319679	-6.381622	0.016431
18	1	0	-2.847076	-6.321041	-0.029271
19	1	0	-5.473746	-2.093845	0.033208
20	1	0	-6.614498	-4.241768	0.056392
21	1	0	2.606870	-1.725703	0.026340
22	1	0	1.368699	0.447373	0.068415
23	1	0	-1.061359	0.498168	0.041418
24	6	0	-3.525350	-0.372734	-0.080527
25	1	0	-3.776804	-0.025049	0.931808
26	1	0	-2.960233	0.424409	-0.568608
27	1	0	-4.462645	-0.469991	-0.633872

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370517	0.000000			
3	C	2.441903	1.431357	0.000000		
4	C	2.855769	2.486407	1.447625	0.000000	
5	C	2.431810	2.805664	2.459457	1.435276	0.000000
6	C	1.424381	2.417189	2.819426	2.453191	1.373182
7	C	3.716378	2.462880	1.397994	2.458545	3.742533
8	C	4.273281	3.781498	2.480883	1.417758	2.506674
9	C	5.109288	4.273160	2.841971	2.451296	3.787181
10	C	4.880076	3.749571	2.438524	2.840924	4.273867
11	C	6.158714	4.924654	3.749163	4.272186	5.705099
12	H	6.340687	5.014910	4.070380	4.889931	6.288424
13	C	7.320941	6.158954	4.880127	5.109093	6.527153
14	C	7.475031	6.485880	5.087907	4.904189	6.224818
15	C	6.527841	5.706261	4.275090	3.788300	5.012254
16	H	4.048591	2.682606	2.151309	3.445225	4.609149
17	H	1.086887	2.137412	3.429900	3.942544	3.408918
18	H	2.139380	1.087879	2.168891	3.462137	3.893496
19	H	3.406406	3.889334	3.449243	2.184767	1.084164
20	H	2.176641	3.395782	3.906470	3.434924	2.132496
21	H	8.275270	7.059740	5.846403	6.170865	7.595519
22	H	8.515925	7.558431	6.151480	5.873635	7.138047
23	H	7.005708	6.351508	4.938511	4.163030	5.180154

This journal is © The Royal Society of Chemistry 2014

24	C	5.215530	5.026514	3.870939	2.540536	2.958552
25	H	5.578156	5.468028	4.374238	3.059728	3.306299
26	H	6.162471	5.866228	4.619129	3.414552	3.969055
27	H	5.013250	5.073637	4.126229	2.712167	2.644142
		6	7	8	9	10
6	C	0.000000				
7	C	4.217333	0.000000			
8	C	3.759564	2.844313	0.000000		
9	C	4.903717	2.459409	1.418099	0.000000	
10	C	5.087355	1.397990	2.480739	1.448083	0.000000
11	C	6.485288	2.462228	3.781843	2.487103	1.431414
12	H	6.886965	2.675519	4.645854	3.462722	2.168846
13	C	7.474787	3.715924	4.274504	2.856687	2.441989
14	C	7.354993	4.217142	3.761250	2.453741	2.819250
15	C	6.225184	3.742916	2.508717	1.435583	2.459351
16	H	4.844178	1.088487	3.932765	3.445968	2.151278
17	H	2.179743	4.597947	5.360125	6.171187	5.846584
18	H	3.411771	2.676742	4.645957	4.891546	4.071544
19	H	2.118771	4.632637	2.753218	4.160112	4.936049
20	H	1.087100	5.304328	4.636809	5.872929	6.150855
21	H	8.506558	4.597305	5.361350	3.943458	3.430009
22	H	8.323387	5.304128	4.638678	3.435345	3.906293
23	H	6.491395	4.633733	2.756771	2.185323	3.449407
24	C	4.331509	4.359119	1.514936	2.544946	3.873778
25	H	4.628137	4.883882	2.176611	3.094802	4.398777
26	H	5.333147	4.870384	2.173261	2.704544	4.124825
27	H	3.946073	4.864111	2.171497	3.403460	4.607732
		11	12	13	14	15
11	C	0.000000				
12	H	1.087876	0.000000			
13	C	1.370389	2.139224	0.000000		
14	C	2.416859	3.411472	1.424333	0.000000	
15	C	2.805455	3.893284	2.431853	1.373119	0.000000
16	H	2.681446	2.432813	4.047378	4.843330	4.609071
17	H	7.059735	7.131565	8.275425	8.506898	7.596269
18	H	5.015578	4.867183	6.341421	6.887977	6.289977
19	H	6.349136	7.046964	7.003645	6.489448	5.178397
20	H	7.557803	7.973568	8.515625	8.323284	7.138248
21	H	2.137380	2.473707	1.086885	2.179769	3.408964
22	H	3.395470	4.303702	2.176555	1.087101	2.132360
23	H	3.888887	4.976746	3.405741	2.117810	1.083969
24	C	5.031715	5.991085	5.223878	4.341885	2.968962
25	H	5.508420	6.470179	5.637657	4.700037	3.374594
26	H	5.068832	6.097767	5.002463	3.928664	2.624717
27	H	5.851828	6.753443	6.146782	5.318300	3.956699
		16	17	18	19	20
16	H	0.000000				
17	H	4.745455	0.000000			
18	H	2.434760	2.473767	0.000000		
19	H	5.572805	4.290577	4.977197	0.000000	
20	H	5.912608	2.501425	4.303973	2.432164	0.000000
21	H	4.743914	9.192815	7.132023	8.089001	9.558509

22	H	5.911680	9.558885	7.974569	7.299184	9.258489
23	H	5.573326	8.091070	7.049496	5.117398	7.300997
24	C	5.447508	6.271821	5.987073	2.602192	4.952878
25	H	5.955497	6.604876	6.436426	2.822589	5.157477
26	H	5.938055	7.227123	6.767923	3.608536	5.959654
27	H	5.931101	6.008725	6.100032	2.025888	4.396957

		21	22	23	24	25
21	H	0.000000				
22	H	2.501419	0.000000			
23	H	4.289724	2.430739	0.000000		
24	C	6.280610	4.964522	2.616217	0.000000	
25	H	6.668088	5.238782	2.905201	1.099516	0.000000
26	H	5.997464	4.375612	1.995819	1.092254	1.766366
27	H	7.210460	5.944690	3.600291	1.092782	1.766269

		26	27
26	H	0.000000	
27	H	1.749701	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.659562	-0.994969	0.020335
2	6	0	-2.461288	-1.659430	-0.010439
3	6	0	-1.218403	-0.949543	-0.019267
4	6	0	-1.225350	0.498039	-0.010613
5	6	0	-2.505633	1.145610	0.028731
6	6	0	-3.676932	0.429085	0.045393
7	6	0	0.001349	-1.632498	-0.032215
8	6	0	-0.000545	1.211814	-0.030988
9	6	0	1.225945	0.500248	-0.010961
10	6	0	1.220121	-0.947795	-0.019853
11	6	0	2.463366	-1.657174	-0.011427
12	1	0	2.434786	-2.744585	-0.025400
13	6	0	3.661378	-0.992526	0.019798
14	6	0	3.678061	0.431469	0.045974
15	6	0	2.506621	1.147649	0.029527
16	1	0	0.002151	-2.720931	-0.042954
17	1	0	-4.595402	-1.547639	0.029440
18	1	0	-2.432396	-2.746842	-0.023874
19	1	0	-2.557721	2.228069	0.060045
20	1	0	-4.628794	0.953049	0.080144
21	1	0	4.597413	-1.544864	0.028830
22	1	0	4.629695	0.955791	0.081573
23	1	0	2.559676	2.229819	0.062401
24	6	0	-0.006290	2.726558	-0.054479

```
     25          1           0       -0.045984    3.149356    0.959721
     26          1           0        0.884037    3.130040   -0.541857
     27          1           0       -0.864487    3.119516   -0.605165
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3931346      0.4478866
0.3397321
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8695425468 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
```

This journal is © The Royal Society of Chemistry 2014

```
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860565916     A.U. after   10 cycles
             Convg  =    0.6177D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000179261   -0.000088659   -0.000014659
      2        6          -0.000173886   -0.000009878    0.000044326
      3        6          -0.000177320    0.000127949    0.000014671
      4        6           0.000126345   -0.000093242   -0.000081939
      5        6          -0.000070642   -0.000084997    0.000100689
      6        6           0.000036450    0.000140703   -0.000009854
      7        6           0.000046965   -0.000017637   -0.000011592
      8        6           0.000139000    0.000184392   -0.000095848
      9        6          -0.000162524   -0.000065995   -0.000007366
     10        6          -0.000080250    0.000132490    0.000006621
     11        6           0.000120662    0.000156522    0.000035290
     12        1          -0.000036274   -0.000067318   -0.000001751
     13        6           0.000018647   -0.000233573   -0.000006016
     14        6          -0.000190206    0.000044706   -0.000020033
     15        6           0.000148908   -0.000074765    0.000072850
     16        1           0.000022507   -0.000025380   -0.000007190
     17        1          -0.000054190    0.000005365    0.000006013
     18        1           0.000066484   -0.000007896   -0.000006639
     19        1          -0.000017132   -0.000004137    0.000011517
     20        1          -0.000028607   -0.000028204   -0.000004563
     21        1           0.000021856    0.000048425   -0.000001841
     22        1           0.000023322    0.000017187   -0.000000367
     23        1          -0.000002666    0.000058555   -0.000001821
     24        6           0.000194438   -0.000106137   -0.000024095
     25        1           0.000001407   -0.000013867   -0.000045748
```

```
     26        1          -0.000164866   -0.000036162    0.000075309
     27        1           0.000012310    0.000041554   -0.000025963
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000233573 RMS     0.000085693


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000157263 RMS     0.000046240
 Search for a local minimum.
 Step number  17 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17
 DE= -4.33D-07 DEPred=-5.90D-07 R= 7.33D-01
 Trust test= 7.33D-01 RLast= 5.00D-02 DXMaxT set to 5.00D-02
 Use linear search instead of GDIIS.
 Linear search step of   0.100 exceeds DXMaxT=   0.050 scaled by
0.999
 Quartic linear search produced a step of  1.99838.
 Iteration  1 RMS(Cart)=  0.01154509 RMS(Int)=  0.00020916
 Iteration  2 RMS(Cart)=  0.00021697 RMS(Int)=  0.00000182
 Iteration  3 RMS(Cart)=  0.00000006 RMS(Int)=  0.00000182
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.58990  -0.00012   0.00049   0.00000   0.00049
2.59040
    R2        2.69169   0.00006  -0.00038   0.00000  -0.00038
2.69131
    R3        2.05392   0.00002  -0.00001   0.00000  -0.00001
2.05391
    R4        2.70487   0.00003  -0.00034   0.00000  -0.00034
2.70453
    R5        2.05579   0.00004  -0.00006   0.00000  -0.00006
2.05573
    R6        2.73561  -0.00013   0.00007   0.00000   0.00007
2.73568
    R7        2.64183   0.00003  -0.00013   0.00000  -0.00013
2.64169
    R8        2.71228   0.00008  -0.00053   0.00000  -0.00053
2.71175
    R9        2.67917   0.00009  -0.00028   0.00000  -0.00028
2.67889
```

R10	2.59494	-0.00005	0.00034	0.00000	0.00034
2.59528					
R11	2.04877	0.00001	0.00010	0.00000	0.00010
2.04887					
R12	2.05432	0.00003	-0.00008	0.00000	-0.00008
2.05425					
R13	2.64182	0.00000	-0.00007	0.00000	-0.00007
2.64175					
R14	2.05694	0.00003	-0.00004	0.00000	-0.00004
2.05691					
R15	2.67982	-0.00010	0.00068	0.00000	0.00068
2.68050					
R16	2.86281	-0.00012	0.00103	0.00000	0.00103
2.86384					
R17	2.73648	-0.00006	0.00095	0.00000	0.00095
2.73743					
R18	2.71286	0.00002	0.00015	0.00000	0.00015
2.71300					
R19	2.70498	0.00004	-0.00026	0.00000	-0.00026
2.70472					
R20	2.05579	0.00004	-0.00007	0.00000	-0.00007
2.05572					
R21	2.58966	-0.00013	0.00024	0.00000	0.00024
2.58990					
R22	2.69160	0.00009	-0.00054	0.00000	-0.00054
2.69106					
R23	2.05391	0.00002	-0.00002	0.00000	-0.00002
2.05390					
R24	2.59482	-0.00009	0.00025	0.00000	0.00025
2.59507					
R25	2.05432	0.00003	-0.00007	0.00000	-0.00007
2.05425					
R26	2.04840	0.00005	-0.00037	0.00000	-0.00037
2.04804					
R27	2.07778	-0.00005	-0.00009	0.00000	-0.00009
2.07769					
R28	2.06406	-0.00015	-0.00043	0.00000	-0.00043
2.06363					
R29	2.06506	0.00000	0.00055	0.00000	0.00055
2.06561					
A1	2.08952	-0.00004	0.00050	0.00000	0.00050
2.09002					
A2	2.10189	0.00007	-0.00097	0.00000	-0.00097
2.10092					
A3	2.09177	-0.00003	0.00047	0.00000	0.00047
2.09224					
A4	2.11634	0.00000	-0.00003	0.00000	-0.00003
2.11631					
A5	2.10379	0.00005	-0.00081	0.00000	-0.00081
2.10298					
A6	2.06304	-0.00005	0.00084	0.00000	0.00084
2.06388					

This journal is © The Royal Society of Chemistry 2014

A7	2.08488	0.00008	-0.00066	0.00000	-0.00066
2.08422					
A8	2.11226	-0.00005	0.00098	0.00000	0.00098
2.11324					
A9	2.08605	-0.00003	-0.00032	0.00000	-0.00032
2.08573					
A10	2.04386	-0.00007	0.00090	0.00000	0.00089
2.04475					
A11	2.09348	0.00003	0.00050	0.00000	0.00050
2.09398					
A12	2.14582	0.00004	-0.00137	0.00000	-0.00137
2.14445					
A13	2.12442	0.00001	-0.00025	0.00000	-0.00025
2.12418					
A14	2.08762	0.00001	-0.00056	0.00000	-0.00056
2.08706					
A15	2.07105	-0.00002	0.00080	0.00000	0.00080
2.07185					
A16	2.10722	0.00002	-0.00043	0.00000	-0.00043
2.10679					
A17	2.08646	-0.00004	0.00045	0.00000	0.00045
2.08691					
A18	2.08950	0.00002	-0.00002	0.00000	-0.00002
2.08948					
A19	2.11917	-0.00001	0.00019	0.00000	0.00019
2.11936					
A20	2.08201	0.00001	-0.00008	0.00000	-0.00008
2.08193					
A21	2.08197	0.00000	-0.00009	0.00000	-0.00009
2.08187					
A22	2.08789	-0.00001	0.00018	0.00000	0.00018
2.08806					
A23	2.09478	-0.00010	-0.00305	0.00000	-0.00305
2.09173					
A24	2.10042	0.00011	0.00292	0.00000	0.00292
2.10334					
A25	2.09231	-0.00001	-0.00076	0.00000	-0.00076
2.09155					
A26	2.14799	0.00008	0.00100	0.00000	0.00100
2.14899					
A27	2.04285	-0.00007	-0.00023	0.00000	-0.00023
2.04262					
A28	2.08670	0.00003	0.00035	0.00000	0.00034
2.08705					
A29	2.11125	-0.00009	-0.00010	0.00000	-0.00010
2.11116					
A30	2.08522	0.00007	-0.00024	0.00000	-0.00024
2.08498					
A31	2.06289	-0.00007	0.00072	0.00000	0.00072
2.06362					
A32	2.11656	0.00000	0.00019	0.00000	0.00018
2.11674					

A33	2.10373	0.00006	-0.00091	0.00000	-0.00091	2.10282
A34	2.08926	-0.00006	0.00024	0.00000	0.00024	2.08950
A35	2.10203	0.00008	-0.00083	0.00000	-0.00083	2.10120
A36	2.09188	-0.00002	0.00059	0.00000	0.00060	2.09248
A37	2.10742	0.00004	-0.00022	0.00000	-0.00022	2.10719
A38	2.08639	-0.00003	0.00034	0.00000	0.00034	2.08673
A39	2.08937	-0.00001	-0.00011	0.00000	-0.00011	2.08926
A40	2.12491	0.00002	0.00028	0.00000	0.00028	2.12520
A41	2.08833	0.00002	0.00026	0.00000	0.00026	2.08859
A42	2.06984	-0.00003	-0.00056	0.00000	-0.00056	2.06929
A43	1.95015	-0.00003	0.00016	0.00000	0.00016	1.95031
A44	1.95324	0.00016	0.00077	0.00000	0.00077	1.95400
A45	1.95017	0.00001	-0.00222	0.00000	-0.00222	1.94795
A46	1.87441	-0.00006	0.00078	0.00000	0.00077	1.87518
A47	1.87360	-0.00001	-0.00014	0.00000	-0.00015	1.87346
A48	1.85714	-0.00009	0.00075	0.00000	0.00075	1.85790
D1	-0.00102	-0.00001	0.00072	0.00000	0.00072	-0.00031
D2	3.13524	-0.00001	0.00075	0.00000	0.00075	3.13599
D3	-3.13865	0.00000	-0.00012	0.00000	-0.00012	-3.13877
D4	-0.00238	0.00000	-0.00009	0.00000	-0.00009	-0.00247
D5	0.00877	0.00001	-0.00053	0.00000	-0.00053	0.00824
D6	-3.13063	0.00001	-0.00118	0.00000	-0.00118	-3.13181
D7	-3.13677	-0.00001	0.00030	0.00000	0.00030	-3.13647
D8	0.00702	0.00000	-0.00036	0.00000	-0.00035	0.00667
D9	-0.01218	0.00000	0.00077	0.00000	0.00077	-0.01141
D10	3.12617	-0.00001	0.00212	0.00000	0.00212	3.12828

This journal is © The Royal Society of Chemistry 2014

D11	3.13462	-0.00001	0.00074	0.00000	0.00074	3.13536
D12	-0.01022	-0.00002	0.00209	0.00000	0.00209	-0.00813
D13	0.01728	0.00002	-0.00235	0.00000	-0.00235	0.01493
D14	-3.13202	-0.00001	0.00059	0.00000	0.00060	-3.13142
D15	-3.12111	0.00003	-0.00368	0.00000	-0.00368	-3.12479
D16	0.01277	0.00000	-0.00074	0.00000	-0.00074	0.01204
D17	-3.12394	0.00004	-0.00319	0.00000	-0.00319	-3.12713
D18	0.00774	0.00001	-0.00151	0.00000	-0.00151	0.00623
D19	0.01440	0.00002	-0.00184	0.00000	-0.00184	0.01256
D20	-3.13710	0.00000	-0.00016	0.00000	-0.00016	-3.13726
D21	-0.01000	-0.00003	0.00259	0.00000	0.00259	-0.00741
D22	3.11663	-0.00002	0.00222	0.00000	0.00222	3.11885
D23	3.13955	0.00001	-0.00046	0.00000	-0.00046	3.13910
D24	-0.01701	0.00001	-0.00083	0.00000	-0.00082	-0.01783
D25	-0.03961	-0.00003	0.00310	0.00000	0.00310	-0.03651
D26	3.11681	0.00001	-0.00093	0.00000	-0.00092	3.11589
D27	3.09381	-0.00006	0.00623	0.00000	0.00622	3.10004
D28	-0.03296	-0.00003	0.00220	0.00000	0.00221	-0.03075
D29	-0.00296	0.00002	-0.00119	0.00000	-0.00119	-0.00415
D30	3.13643	0.00001	-0.00054	0.00000	-0.00054	3.13590
D31	-3.12972	0.00001	-0.00082	0.00000	-0.00082	-3.13053
D32	0.00967	0.00000	-0.00016	0.00000	-0.00016	0.00951
D33	-0.01421	-0.00002	0.00199	0.00000	0.00199	-0.01222
D34	3.12378	-0.00003	0.00285	0.00000	0.00285	3.12663
D35	3.13728	0.00000	0.00031	0.00000	0.00031	3.13760
D36	-0.00791	-0.00001	0.00117	0.00000	0.00117	-0.00674

This journal is © The Royal Society of Chemistry 2014

D37	0.03977	0.00003	-0.00297	0.00000	-0.00297	0.03680
D38	-3.09256	0.00004	-0.00414	0.00000	-0.00414	-3.09670
D39	-3.11669	-0.00001	0.00102	0.00000	0.00103	-3.11567
D40	0.03417	0.00000	-0.00016	0.00000	-0.00015	0.03402
D41	1.52586	-0.00004	-0.03941	0.00000	-0.03941	1.48645
D42	-2.65452	-0.00003	-0.03776	0.00000	-0.03776	-2.69228
D43	-0.57379	-0.00002	-0.03779	0.00000	-0.03779	-0.61158
D44	-1.60081	-0.00001	-0.04344	0.00000	-0.04344	-1.64425
D45	0.50200	0.00001	-0.04179	0.00000	-0.04179	0.46021
D46	2.58273	0.00001	-0.04182	0.00000	-0.04182	2.54091
D47	-0.01313	-0.00001	0.00044	0.00000	0.00044	-0.01269
D48	3.13201	0.00000	-0.00041	0.00000	-0.00040	3.13160
D49	3.11974	-0.00002	0.00155	0.00000	0.00155	3.12129
D50	-0.01830	-0.00001	0.00071	0.00000	0.00071	-0.01760
D51	-3.13974	0.00001	-0.00008	0.00000	-0.00008	-3.13982
D52	0.01734	-0.00001	0.00103	0.00000	0.00103	0.01836
D53	0.01088	0.00002	-0.00122	0.00000	-0.00122	0.00966
D54	-3.11523	0.00001	-0.00011	0.00000	-0.00011	-3.11535
D55	0.01095	0.00001	-0.00096	0.00000	-0.00096	0.00999
D56	-3.12529	0.00000	-0.00076	0.00000	-0.00076	-3.12605
D57	-3.13424	0.00000	-0.00010	0.00000	-0.00010	-3.13435
D58	0.01271	0.00000	0.00009	0.00000	0.00009	0.01280
D59	0.00121	0.00001	-0.00043	0.00000	-0.00043	0.00078
D60	3.13839	0.00001	-0.00033	0.00000	-0.00033	3.13806
D61	-3.13490	0.00001	-0.00023	0.00000	-0.00023	-3.13514
D62	0.00228	0.00000	-0.00014	0.00000	-0.00014	0.00214

```
   D63       -0.00912   0.00000  -0.00008   0.00000  -0.00008  -
0.00920
   D64        3.13011   0.00000   0.00039   0.00000   0.00039
3.13050
   D65        3.13685   0.00000  -0.00017   0.00000  -0.00017
3.13669
   D66       -0.00710   0.00000   0.00030   0.00000   0.00030  -
0.00680
   D67        0.00276  -0.00001   0.00093   0.00000   0.00093
0.00368
   D68        3.12903   0.00000  -0.00016   0.00000  -0.00016
3.12886
   D69       -3.13648  -0.00001   0.00046   0.00000   0.00046  -
3.13602
   D70       -0.01021   0.00000  -0.00063   0.00000  -0.00063  -
0.01084
         Item               Value     Threshold  Converged?
 Maximum Force            0.000157     0.000450     YES
 RMS     Force            0.000046     0.000300     YES
 Maximum Displacement     0.077448     0.001800     NO
 RMS     Displacement     0.011545     0.001200     NO
 Predicted change in Energy=-9.071854D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792798   -5.429449    0.006481
      2          6           0       -3.422612   -5.397199   -0.017694
      3          6           0       -2.709073   -4.156618   -0.026684
      4          6           0       -3.447637   -2.911531   -0.024329
      5          6           0       -4.879607   -2.999506    0.006179
      6          6           0       -5.528190   -4.209944    0.023472
      7          6           0       -1.311469   -4.128017   -0.035420
      8          6           0       -2.753037   -1.675936   -0.045644
      9          6           0       -1.334763   -1.668094   -0.024196
     10          6           0       -0.606984   -2.920582   -0.026985
     11          6           0        0.824155   -2.903162   -0.017690
     12          1           0        1.350521   -3.855134   -0.026927
     13          6           0        1.521299   -1.723498    0.008811
     14          6           0        0.815654   -0.486731    0.028556
     15          6           0       -0.557250   -0.461699    0.010490
     16          1           0       -0.759741   -5.066273   -0.041277
     17          1           0       -5.320075   -6.379818    0.015676
     18          1           0       -2.848768   -6.321347   -0.025612
     19          1           0       -5.471226   -2.091255    0.030440
     20          1           0       -6.614493   -4.238900    0.051880
     21          1           0        2.608123   -1.727217    0.018868
```

22	1	0	1.371092	0.447185	0.060042
23	1	0	-1.058389	0.498842	0.038582
24	6	0	-3.529311	-0.374743	-0.076902
25	1	0	-3.817788	-0.048199	0.932543
26	1	0	-2.952382	0.434104	-0.530158
27	1	0	-4.446682	-0.467291	-0.663988

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370778	0.000000			
3	C	2.441948	1.431175	0.000000		
4	C	2.854876	2.485803	1.447661	0.000000	
5	C	2.431493	2.805768	2.459919	1.434994	0.000000
6	C	1.424178	2.417587	2.820068	2.452930	1.373360
7	C	3.716871	2.463344	1.397924	2.458287	3.742576
8	C	4.272259	3.781126	2.481143	1.417610	2.505359
9	C	5.109475	4.273802	2.842795	2.451606	3.786753
10	C	4.880222	3.749864	2.438557	2.840668	4.273480
11	C	6.158966	4.924962	3.748990	4.271805	5.704625
12	H	6.341920	5.016059	4.070773	4.890062	6.288695
13	C	7.321332	6.159468	4.880305	5.109094	6.526852
14	C	7.475672	6.486736	5.088695	4.904906	6.224993
15	C	6.528279	5.707036	4.275997	3.789093	5.012310
16	H	4.049657	2.683459	2.151181	3.444994	4.609454
17	H	1.086880	2.137059	3.429541	3.941655	3.408902
18	H	2.139104	1.087846	2.169232	3.462007	3.893577
19	H	3.406520	3.889525	3.449417	2.184209	1.084215
20	H	2.176705	3.396263	3.907077	3.434632	2.132608
21	H	8.275282	7.059736	5.846079	6.170631	7.595063
22	H	8.516527	7.559264	6.152257	5.874372	7.138195
23	H	7.006530	6.352639	4.939870	4.164505	5.180849
24	C	5.210893	5.023938	3.870127	2.538647	2.952894
25	H	5.546718	5.447102	4.362164	3.041593	3.270447
26	H	6.168984	5.872635	4.624653	3.419710	3.973856
27	H	5.019197	5.076457	4.127538	2.716903	2.654932

		6	7	8	9	10
6	C	0.000000				
7	C	4.217929	0.000000			
8	C	3.758650	2.844455	0.000000		
9	C	4.903887	2.460058	1.418458	0.000000	
10	C	5.087560	1.397951	2.480934	1.448584	0.000000
11	C	6.485496	2.462005	3.781953	2.487239	1.431275
12	H	6.888040	2.675953	4.646336	3.463221	2.169150
13	C	7.475154	3.715944	4.274948	2.856790	2.442106
14	C	7.355726	4.217547	3.762349	2.454118	2.819684
15	C	6.225734	3.743373	2.509782	1.435660	2.459672
16	H	4.845162	1.088468	3.932891	3.446529	2.151169
17	H	2.179845	4.598059	5.359100	6.171276	5.846483
18	H	3.411706	2.678448	4.646440	4.893360	4.073180
19	H	2.119466	4.632097	2.750788	4.158411	4.934768
20	H	1.087060	5.304902	4.635638	5.872851	6.150963

This journal is © The Royal Society of Chemistry 2014

21	H	8.506677	4.596736	5.361794	3.943564	3.429743
22	H	8.324079	5.304500	4.639748	3.435572	3.906689
23	H	6.492458	4.634366	2.758366	2.185391	3.449714
24	C	4.326010	4.359772	1.515480	2.547857	3.876052
25	H	4.590425	4.885029	2.177171	3.115257	4.413677
26	H	5.339333	4.873429	2.174112	2.700357	4.124075
27	H	3.955972	4.860615	2.170623	3.396366	4.600836

		11	12	13	14	15
11	C	0.000000				
12	H	1.087841	0.000000			
13	C	1.370518	2.138765	0.000000		
14	C	2.416889	3.411056	1.424050	0.000000	
15	C	2.805319	3.893121	2.431564	1.373251	0.000000
16	H	2.681106	2.433160	4.047197	4.843445	4.609315
17	H	7.059732	7.132510	8.275613	8.507398	7.596622
18	H	5.017410	4.869931	6.343413	6.890114	6.291886
19	H	6.347703	7.046332	7.002223	6.488403	5.177163
20	H	7.557944	7.974643	8.515881	8.323845	7.138568
21	H	2.136990	2.472183	1.086877	2.179873	3.408987
22	H	3.395587	4.303247	2.176477	1.087061	2.132377
23	H	3.888543	4.976369	3.405066	2.117426	1.083775
24	C	5.034786	5.994028	5.228302	4.347687	2.974617
25	H	5.531852	6.490359	5.671487	4.741128	3.413543
26	H	5.065787	6.096374	4.995954	3.918953	2.613699
27	H	5.842336	6.744693	6.135757	5.307746	3.947484

		16	17	18	19	20
16	H	0.000000				
17	H	4.746082	0.000000			
18	H	2.437106	2.472344	0.000000		
19	H	5.572609	4.291251	4.977360	0.000000	
20	H	5.913658	2.502071	4.303868	2.433084	0.000000
21	H	4.742934	9.192553	7.133419	8.087555	9.558572
22	H	5.911763	9.559376	7.976690	7.298074	9.258998
23	H	5.573695	8.091876	7.051564	5.116816	7.301826
24	C	5.448141	6.267084	5.985639	2.594027	4.946377
25	H	5.956597	6.571675	6.419459	2.778799	5.114597
26	H	5.941450	7.234186	6.775059	3.610580	5.965467
27	H	5.927220	6.015209	6.101707	2.041858	4.408731

		21	22	23	24	25
21	H	0.000000				
22	H	2.501993	0.000000			
23	H	4.289410	2.430125	0.000000		
24	C	6.285416	4.970741	2.623345	0.000000	
25	H	6.704196	5.284993	2.951729	1.099468	0.000000
26	H	5.990989	4.363592	1.978602	1.092027	1.766647
27	H	7.198888	5.933547	3.592707	1.093071	1.766368

		26	27
26	H	0.000000	
27	H	1.750245	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75

This journal is © The Royal Society of Chemistry 2014

```
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.658767   -0.995811    0.017920
      2          6           0       -2.460307   -1.660618   -0.009634
      3          6           0       -1.217470   -0.950990   -0.016259
      4          6           0       -1.225192    0.496626   -0.007827
      5          6           0       -2.505128    1.144565    0.026029
      6          6           0       -3.676679    0.428069    0.040893
      7          6           0        0.002809   -1.632872   -0.028456
      8          6           0       -0.001222    1.211579   -0.026745
      9          6           0        1.226409    0.501210   -0.008880
     10          6           0        1.221084   -0.947337   -0.017744
     11          6           0        2.464652   -1.655896   -0.012032
     12          1           0        2.437485   -2.743310   -0.025818
     13          6           0        3.662563   -0.990685    0.016670
     14          6           0        3.679045    0.433037    0.042379
     15          6           0        2.507180    1.148817    0.027893
     16          1           0        0.004459   -2.721289   -0.038879
     17          1           0       -4.594176   -1.549223    0.025253
     18          1           0       -2.432443   -2.748036   -0.022128
     19          1           0       -2.556358    2.227185    0.054857
     20          1           0       -4.628544    0.952176    0.071968
     21          1           0        4.598376   -1.543408    0.023949
     22          1           0        4.630452    0.957845    0.075600
     23          1           0        2.560453    2.230790    0.060498
     24          6           0       -0.013130    2.726809   -0.051641
     25          1           0       -0.096431    3.150154    0.959631
     26          1           0        0.893348    3.134879   -0.503635
     27          1           0       -0.851697    3.113225   -0.636698
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3931618      0.4478409
0.3396931
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8403843586 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
```

```
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860565740     A.U. after   11 cycles
            Convg  =    0.4123D-08             -V/T =  2.0100
```

This journal is © The Royal Society of Chemistry 2014

```
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000378959   -0.000222463   -0.000029602
      2        6          -0.000367642   -0.000061947    0.000129363
      3        6          -0.000391396    0.000310959    0.000026141
      4        6           0.000295016   -0.000213425   -0.000251433
      5        6          -0.000154409   -0.000176189    0.000312689
      6        6           0.000078512    0.000325146   -0.000048792
      7        6           0.000118151   -0.000055027   -0.000032119
      8        6           0.000312587    0.000463841   -0.000292668
      9        6          -0.000393079   -0.000140899   -0.000018801
     10        6          -0.000213960    0.000292288    0.000000077
     11        6           0.000298090    0.000313409    0.000104616
     12        1          -0.000104497   -0.000130779   -0.000005385
     13        6           0.000078456   -0.000520159   -0.000003640
     14        6          -0.000440090    0.000108129   -0.000077009
     15        6           0.000320016   -0.000184525    0.000236489
     16        1           0.000039219   -0.000034824   -0.000013532
     17        1          -0.000119844    0.000029641    0.000012639
     18        1           0.000140714    0.000010160   -0.000018988
     19        1          -0.000032566   -0.000017301    0.000023900
     20        1          -0.000052560   -0.000060449   -0.000015526
     21        1           0.000032891    0.000115807   -0.000009304
     22        1           0.000040057    0.000031688   -0.000003120
     23        1          -0.000008685    0.000135526   -0.000014433
     24        6           0.000521443   -0.000323777   -0.000024765
     25        1           0.000006769   -0.000018617   -0.000057308
     26        1          -0.000347372   -0.000044197    0.000149721
     27        1          -0.000034781    0.000067984   -0.000079210
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000521443 RMS     0.000202246


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000367496 RMS     0.000106872
 Search for a local minimum.
 Step number  18 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
```

This journal is © The Royal Society of Chemistry 2014

```
                                                          11    12    13    14
15
                                                          16    17    18
     Eigenvalues ---    0.00001   0.01191   0.01586   0.01771
0.01778
     Eigenvalues ---    0.01818   0.01820   0.01857   0.01972
0.01978
     Eigenvalues ---    0.01983   0.02045   0.02071   0.02101
0.02113
     Eigenvalues ---    0.02143   0.02153   0.02216   0.02230
0.02301
     Eigenvalues ---    0.02350   0.02912   0.06627   0.06854
0.12399
     Eigenvalues ---    0.15523   0.15786   0.15989   0.15999
0.16000
     Eigenvalues ---    0.16000   0.16004   0.16018   0.16199
0.16224
     Eigenvalues ---    0.19329   0.21990   0.22119   0.22392
0.22636
     Eigenvalues ---    0.23425   0.24454   0.24843   0.24984
0.27370
     Eigenvalues ---    0.28351   0.32491   0.33567   0.33623
0.33631
     Eigenvalues ---    0.33681   0.33682   0.33717   0.33846
0.34083
     Eigenvalues ---    0.34142   0.36692   0.37130   0.37353
0.37573
     Eigenvalues ---    0.38432   0.39410   0.39760   0.40494
0.41118
     Eigenvalues ---    0.41832   0.44785   0.45332   0.46999
0.49623
     Eigenvalues ---    0.49832   0.50283   0.51258   0.55228
1.08043
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   6.17D-06 Eigenvector:
                          D44       D46       D45       D41       D43
   1                    0.42967   0.41195   0.41165   0.40528
0.38756
                          D42       D27       A23       A24       A45
   1                    0.38725  -0.03973   0.03257  -0.03113
0.02708
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    18   17
 RFO step:  Lambda=-1.87892556D-06.
 DIIS coeffs:     -0.44907      1.44907
 Iteration  1 RMS(Cart)=  0.00275962 RMS(Int)=  0.00000659
 Iteration  2 RMS(Cart)=  0.00000702 RMS(Int)=  0.00000165
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000165
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                   (DIIS)     (GDIIS)  (Total)
    R1        2.59040  -0.00024  -0.00072   0.00064  -0.00008
2.59032
    R2        2.69131   0.00014   0.00055  -0.00047   0.00009
2.69139
    R3        2.05391   0.00003   0.00002  -0.00009  -0.00007
2.05383
    R4        2.70453   0.00007   0.00050  -0.00040   0.00010
2.70463
    R5        2.05573   0.00007   0.00009  -0.00019  -0.00010
2.05563
    R6        2.73568  -0.00032  -0.00010   0.00003  -0.00007
2.73561
    R7        2.64169   0.00006   0.00019  -0.00012   0.00007
2.64176
    R8        2.71175   0.00015   0.00077  -0.00061   0.00016
2.71191
    R9        2.67889   0.00018   0.00041  -0.00016   0.00025
2.67914
   R10        2.59528  -0.00012  -0.00049   0.00046  -0.00003
2.59525
   R11        2.04887   0.00000  -0.00014   0.00002  -0.00012
2.04875
   R12        2.05425   0.00005   0.00011  -0.00020  -0.00009
2.05416
```

This journal is © The Royal Society of Chemistry 2014

R13	2.64175	0.00000	0.00011	-0.00013	-0.00003
2.64172					
R14	2.05691	0.00005	0.00005	-0.00015	-0.00010
2.05681					
R15	2.68050	-0.00029	-0.00098	0.00076	-0.00023
2.68027					
R16	2.86384	-0.00035	-0.00149	0.00128	-0.00021
2.86363					
R17	2.73743	-0.00014	-0.00137	0.00129	-0.00008
2.73734					
R18	2.71300	0.00001	-0.00021	0.00021	0.00000
2.71301					
R19	2.70472	0.00011	0.00038	-0.00024	0.00014
2.70486					
R20	2.05572	0.00006	0.00010	-0.00020	-0.00010
2.05562					
R21	2.58990	-0.00026	-0.00035	0.00029	-0.00006
2.58984					
R22	2.69106	0.00022	0.00078	-0.00060	0.00018
2.69124					
R23	2.05390	0.00003	0.00002	-0.00009	-0.00007
2.05383					
R24	2.59507	-0.00021	-0.00036	0.00028	-0.00008
2.59499					
R25	2.05425	0.00005	0.00011	-0.00020	-0.00009
2.05416					
R26	2.04804	0.00012	0.00053	-0.00051	0.00003
2.04806					
R27	2.07769	-0.00006	0.00013	-0.00002	0.00011
2.07780					
R28	2.06363	-0.00028	0.00062	-0.00063	-0.00001
2.06362					
R29	2.06561	0.00007	-0.00079	0.00084	0.00004
2.06565					
A1	2.09002	-0.00010	-0.00072	0.00070	-0.00002
2.08999					
A2	2.10092	0.00017	0.00140	-0.00127	0.00014
2.10106					
A3	2.09224	-0.00007	-0.00069	0.00057	-0.00011
2.09213					
A4	2.11631	-0.00001	0.00005	-0.00011	-0.00006
2.11625					
A5	2.10298	0.00013	0.00117	-0.00101	0.00016
2.10314					
A6	2.06388	-0.00013	-0.00122	0.00112	-0.00010
2.06378					
A7	2.08422	0.00018	0.00095	-0.00083	0.00013
2.08435					
A8	2.11324	-0.00011	-0.00142	0.00127	-0.00015
2.11309					
A9	2.08573	-0.00008	0.00046	-0.00044	0.00002
2.08575					

This journal is © The Royal Society of Chemistry 2014

A10	2.04475	-0.00015	-0.00129	0.00120	-0.00009
2.04466					
A11	2.09398	0.00008	-0.00072	0.00064	-0.00008
2.09390					
A12	2.14445	0.00007	0.00199	-0.00183	0.00016
2.14461					
A13	2.12418	0.00001	0.00036	-0.00040	-0.00004
2.12413					
A14	2.08706	0.00003	0.00081	-0.00075	0.00006
2.08712					
A15	2.07185	-0.00005	-0.00116	0.00114	-0.00002
2.07183					
A16	2.10679	0.00006	0.00062	-0.00054	0.00008
2.10687					
A17	2.08691	-0.00009	-0.00065	0.00054	-0.00012
2.08679					
A18	2.08948	0.00003	0.00003	0.00000	0.00004
2.08952					
A19	2.11936	-0.00003	-0.00027	0.00021	-0.00006
2.11930					
A20	2.08193	0.00003	0.00012	-0.00007	0.00005
2.08198					
A21	2.08187	0.00000	0.00014	-0.00013	0.00000
2.08188					
A22	2.08806	-0.00002	-0.00026	0.00021	-0.00005
2.08802					
A23	2.09173	-0.00023	0.00443	-0.00418	0.00025
2.09198					
A24	2.10334	0.00025	-0.00423	0.00400	-0.00023
2.10311					
A25	2.09155	-0.00002	0.00111	-0.00105	0.00006
2.09161					
A26	2.14899	0.00016	-0.00145	0.00131	-0.00014
2.14885					
A27	2.04262	-0.00015	0.00033	-0.00025	0.00008
2.04270					
A28	2.08705	0.00006	-0.00050	0.00051	0.00002
2.08706					
A29	2.11116	-0.00021	0.00014	-0.00019	-0.00004
2.11111					
A30	2.08498	0.00015	0.00035	-0.00033	0.00003
2.08501					
A31	2.06362	-0.00016	-0.00105	0.00091	-0.00014
2.06348					
A32	2.11674	0.00000	-0.00027	0.00019	-0.00007
2.11667					
A33	2.10282	0.00016	0.00132	-0.00110	0.00021
2.10303					
A34	2.08950	-0.00014	-0.00034	0.00032	-0.00002
2.08948					
A35	2.10120	0.00019	0.00120	-0.00106	0.00014
2.10134					

```
   A36        2.09248  -0.00005  -0.00086   0.00074  -0.00012
2.09236
   A37        2.10719   0.00010   0.00032  -0.00025   0.00008
2.10727
   A38        2.08673  -0.00007  -0.00049   0.00043  -0.00006
2.08667
   A39        2.08926  -0.00003   0.00017  -0.00019  -0.00002
2.08924
   A40        2.12520   0.00004  -0.00041   0.00031  -0.00010
2.12510
   A41        2.08859   0.00004  -0.00037   0.00028  -0.00009
2.08850
   A42        2.06929  -0.00007   0.00081  -0.00061   0.00020
2.06948
   A43        1.95031  -0.00007  -0.00024   0.00030   0.00006
1.95037
   A44        1.95400   0.00037  -0.00111   0.00095  -0.00016
1.95384
   A45        1.94795   0.00001   0.00322  -0.00348  -0.00026
1.94769
   A46        1.87518  -0.00013  -0.00112   0.00119   0.00007
1.87525
   A47        1.87346  -0.00001   0.00021   0.00000   0.00021
1.87367
   A48        1.85790  -0.00018  -0.00109   0.00119   0.00010
1.85800
    D1       -0.00031  -0.00004  -0.00104   0.00061  -0.00043  -
0.00074
    D2        3.13599  -0.00003  -0.00108   0.00056  -0.00053
3.13546
    D3       -3.13877  -0.00001   0.00017  -0.00015   0.00001  -
3.13875
    D4       -0.00247   0.00000   0.00012  -0.00020  -0.00008  -
0.00255
    D5        0.00824   0.00001   0.00076  -0.00040   0.00036
0.00860
    D6       -3.13181   0.00002   0.00171  -0.00091   0.00080  -
3.13101
    D7       -3.13647  -0.00002  -0.00043   0.00035  -0.00008  -
3.13655
    D8        0.00667   0.00000   0.00051  -0.00016   0.00035
0.00702
    D9       -0.01141   0.00000  -0.00111   0.00065  -0.00046  -
0.01187
   D10        3.12828  -0.00004  -0.00307   0.00184  -0.00123
3.12705
   D11        3.13536  -0.00001  -0.00108   0.00071  -0.00037
3.13499
   D12       -0.00813  -0.00005  -0.00304   0.00189  -0.00114  -
0.00927
   D13        0.01493   0.00006   0.00340  -0.00202   0.00138
0.01631
```

This journal is © The Royal Society of Chemistry 2014

D14	-3.13142	-0.00004	-0.00086	0.00046	-0.00040	-3.13183
D15	-3.12479	0.00010	0.00533	-0.00319	0.00214	-3.12266
D16	0.01204	0.00000	0.00107	-0.00071	0.00036	0.01239
D17	-3.12713	0.00010	0.00462	-0.00241	0.00221	-3.12492
D18	0.00623	0.00003	0.00219	-0.00101	0.00118	0.00741
D19	0.01256	0.00006	0.00266	-0.00122	0.00144	0.01400
D20	-3.13726	-0.00001	0.00023	0.00017	0.00041	-3.13685
D21	-0.00741	-0.00009	-0.00375	0.00227	-0.00148	-0.00889
D22	3.11885	-0.00006	-0.00322	0.00202	-0.00120	3.11765
D23	3.13910	0.00001	0.00066	-0.00030	0.00036	3.13946
D24	-0.01783	0.00005	0.00119	-0.00055	0.00064	-0.01720
D25	-0.03651	-0.00007	-0.00449	0.00230	-0.00219	-0.03870
D26	3.11589	0.00004	0.00133	-0.00100	0.00032	3.11621
D27	3.10004	-0.00017	-0.00902	0.00494	-0.00407	3.09596
D28	-0.03075	-0.00006	-0.00320	0.00164	-0.00156	-0.03232
D29	-0.00415	0.00006	0.00173	-0.00110	0.00063	-0.00352
D30	3.13590	0.00004	0.00078	-0.00058	0.00019	3.13609
D31	-3.13053	0.00002	0.00118	-0.00083	0.00035	-3.13018
D32	0.00951	0.00001	0.00024	-0.00032	-0.00008	0.00943
D33	-0.01222	-0.00006	-0.00288	0.00151	-0.00137	-0.01359
D34	3.12663	-0.00008	-0.00413	0.00220	-0.00193	3.12469
D35	3.13760	0.00001	-0.00045	0.00011	-0.00034	3.13726
D36	-0.00674	-0.00001	-0.00170	0.00080	-0.00090	-0.00764
D37	0.03680	0.00007	0.00430	-0.00204	0.00226	0.03906
D38	-3.09670	0.00011	0.00600	-0.00304	0.00297	-3.09373
D39	-3.11567	-0.00004	-0.00149	0.00123	-0.00026	-3.11593

This journal is © The Royal Society of Chemistry 2014

D40	0.03402	0.00000	0.00022	0.00023	0.00044	0.03446
D41	1.48645	-0.00011	0.05711	-0.05112	0.00599	1.49244
D42	-2.69228	-0.00007	0.05472	-0.04871	0.00601	-2.68627
D43	-0.61158	-0.00005	0.05477	-0.04892	0.00585	-0.60573
D44	-1.64425	0.00000	0.06294	-0.05442	0.00852	-1.63573
D45	0.46021	0.00004	0.06055	-0.05201	0.00854	0.46876
D46	2.54091	0.00006	0.06060	-0.05222	0.00838	2.54929
D47	-0.01269	-0.00001	-0.00064	0.00014	-0.00051	-0.01320
D48	3.13160	0.00001	0.00059	-0.00054	0.00005	3.13165
D49	3.12129	-0.00005	-0.00225	0.00108	-0.00117	3.12012
D50	-0.01760	-0.00002	-0.00102	0.00041	-0.00061	-0.01821
D51	-3.13982	0.00002	0.00011	0.00006	0.00017	-3.13965
D52	0.01836	-0.00003	-0.00149	0.00109	-0.00040	0.01797
D53	0.00966	0.00006	0.00177	-0.00091	0.00086	0.01051
D54	-3.11535	0.00001	0.00017	0.00012	0.00029	-3.11506
D55	0.00999	0.00003	0.00139	-0.00077	0.00062	0.01061
D56	-3.12605	0.00001	0.00111	-0.00050	0.00061	-3.12544
D57	-3.13435	0.00000	0.00015	-0.00009	0.00006	-3.13429
D58	0.01280	-0.00002	-0.00014	0.00019	0.00005	0.01285
D59	0.00078	0.00003	0.00062	-0.00031	0.00031	0.00109
D60	3.13806	0.00002	0.00048	-0.00024	0.00024	3.13830
D61	-3.13514	0.00001	0.00034	-0.00003	0.00030	-3.13483
D62	0.00214	0.00001	0.00020	0.00004	0.00024	0.00238
D63	-0.00920	0.00000	0.00011	-0.00019	-0.00008	-0.00928
D64	3.13050	-0.00001	-0.00057	0.00009	-0.00048	3.13002
D65	3.13669	0.00001	0.00024	-0.00026	-0.00002	3.13667

```
   D66       -0.00680   0.00000  -0.00044   0.00002  -0.00042  -
0.00721
   D67        0.00368  -0.00005  -0.00134   0.00082  -0.00052
0.00316
   D68        3.12886   0.00000   0.00023  -0.00020   0.00003
3.12890
   D69       -3.13602  -0.00003  -0.00066   0.00054  -0.00012  -
3.13614
   D70       -0.01084   0.00001   0.00091  -0.00048   0.00043  -
0.01040
         Item               Value     Threshold  Converged?
 Maximum Force            0.000367     0.000450     YES
 RMS     Force            0.000107     0.000300     YES
 Maximum Displacement     0.016530     0.001800     NO
 RMS     Displacement     0.002760     0.001200     NO
 Predicted change in Energy=-1.294885D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792699   -5.429600    0.007477
      2          6           0       -3.422592   -5.397274   -0.018688
      3          6           0       -2.709198   -4.156559   -0.029066
      4          6           0       -3.447743   -2.911504   -0.026588
      5          6           0       -4.879719   -2.999584    0.007221
      6          6           0       -5.528126   -4.210081    0.025712
      7          6           0       -1.311560   -4.127989   -0.038353
      8          6           0       -2.753001   -1.675856   -0.048779
      9          6           0       -1.334874   -1.668113   -0.025625
     10          6           0       -0.607112   -2.920558   -0.028633
     11          6           0        0.824089   -2.903184   -0.017542
     12          1           0        1.350284   -3.855187   -0.027037
     13          6           0        1.521125   -1.723539    0.010942
     14          6           0        0.815325   -0.486762    0.031366
     15          6           0       -0.557519   -0.461698    0.011895
     16          1           0       -0.759840   -5.066186   -0.044687
     17          1           0       -5.320014   -6.379895    0.017724
     18          1           0       -2.848579   -6.321251   -0.027082
     19          1           0       -5.471367   -2.091464    0.032823
     20          1           0       -6.614313   -4.239199    0.056450
     21          1           0        2.607901   -1.727059    0.022121
     22          1           0        1.370685    0.447072    0.064880
     23          1           0       -1.058874    0.498729    0.040526
     24          6           0       -3.528816   -0.374506   -0.079482
     25          1           0       -3.811015   -0.044505    0.930677
     26          1           0       -2.954188    0.432490   -0.538905
     27          1           0       -4.449691   -0.468751   -0.660827
```

This journal is © The Royal Society of Chemistry 2014

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370738	0.000000			
3	C	2.441914	1.431228	0.000000		
4	C	2.854973	2.485909	1.447625	0.000000	
5	C	2.431574	2.805853	2.459893	1.435081	0.000000
6	C	1.424224	2.417576	2.819968	2.452963	1.373345
7	C	3.716803	2.463317	1.397961	2.458303	3.742611
8	C	4.272485	3.781297	2.481168	1.417740	2.505658
9	C	5.109446	4.273787	2.842735	2.451580	3.786796
10	C	4.880137	3.749820	2.438537	2.840647	4.273489
11	C	6.158872	4.924915	3.749026	4.271850	5.704677
12	H	6.341625	5.015820	4.070654	4.889950	6.288575
13	C	7.321153	6.159346	4.880248	5.109044	6.526800
14	C	7.475436	6.486568	5.088548	4.904741	6.224820
15	C	6.528156	5.706968	4.275909	3.788988	5.012215
16	H	4.049535	2.683382	2.151199	3.444968	4.609441
17	H	1.086843	2.137073	3.429544	3.941712	3.408882
18	H	2.139121	1.087794	2.169176	3.461990	3.893608
19	H	3.406521	3.889539	3.449352	2.184273	1.084151
20	H	2.176634	3.396155	3.906926	3.434652	2.132577
21	H	8.275137	7.059673	5.846078	6.170584	7.594998
22	H	8.516213	7.559026	6.152048	5.874152	7.137949
23	H	7.006256	6.352442	4.939647	4.164239	5.180556
24	C	5.211424	5.024259	3.870173	2.538845	2.953555
25	H	5.551149	5.450165	4.363954	3.044340	3.275269
26	H	6.167881	5.871641	4.623778	3.418825	3.973041
27	H	5.017401	5.075196	4.126544	2.715364	2.652607

		6	7	8	9	10
6	C	0.000000				
7	C	4.217852	0.000000			
8	C	3.758878	2.844436	0.000000		
9	C	4.903835	2.460019	1.418338	0.000000	
10	C	5.087455	1.397938	2.480833	1.448539	0.000000
11	C	6.485405	2.462027	3.781915	2.487284	1.431349
12	H	6.887762	2.675811	4.646171	3.463144	2.169086
13	C	7.474962	3.715900	4.274809	2.856771	2.442092
14	C	7.355440	4.217467	3.762089	2.454015	2.819626
15	C	6.225552	3.743366	2.509582	1.435661	2.459694
16	H	4.845041	1.088415	3.932816	3.446437	2.151116
17	H	2.179786	4.598036	5.359288	6.171233	5.846419
18	H	3.411715	2.678238	4.646429	4.893159	4.072946
19	H	2.119389	4.632116	2.751164	4.158512	4.934791
20	H	1.087012	5.304767	4.635896	5.872794	6.150815
21	H	8.506488	4.596770	5.361615	3.943504	3.429770
22	H	8.323713	5.304364	4.639454	3.435440	3.906579
23	H	6.492097	4.634284	2.758053	2.185350	3.449695
24	C	4.326655	4.359650	1.515369	2.547490	3.875736
25	H	4.595590	4.884786	2.177161	3.111573	4.411003
26	H	5.338297	4.873063	2.173895	2.701512	4.124570

27	H	3.953721	4.860593	2.170360	3.397652	4.601787
		11	12	13	14	15
11	C	0.000000				
12	H	1.087788	0.000000			
13	C	1.370487	2.138821	0.000000		
14	C	2.416932	3.411141	1.424145	0.000000	
15	C	2.805451	3.893198	2.431667	1.373210	0.000000
16	H	2.681072	2.432993	4.047121	4.843351	4.609278
17	H	7.059658	7.132253	8.275439	8.507149	7.596476
18	H	5.017147	4.869489	6.343085	6.889766	6.291648
19	H	6.347771	7.046221	7.002200	6.488264	5.177111
20	H	7.557793	7.974287	8.515631	8.323517	7.138365
21	H	2.137014	2.472437	1.086839	2.179852	3.408977
22	H	3.395552	4.303290	2.176487	1.087012	2.132286
23	H	3.888692	4.976464	3.405252	2.117521	1.083788
24	C	5.034464	5.993623	5.227808	4.347004	2.973981
25	H	5.527689	6.486719	5.665402	4.733642	3.406383
26	H	5.066943	6.097103	4.997922	3.921665	2.616673
27	H	5.844059	6.746062	6.138112	5.310352	3.949887
		16	17	18	19	20
16	H	0.000000				
17	H	4.746042	0.000000			
18	H	2.436869	2.472537	0.000000		
19	H	5.572564	4.291128	4.977320	0.000000	
20	H	5.913458	2.501857	4.303798	2.433033	0.000000
21	H	4.742986	9.192428	7.133176	8.087489	9.558308
22	H	5.911612	9.559036	7.976268	7.297868	9.258586
23	H	5.573594	8.091557	7.051223	5.116567	7.301446
24	C	5.447963	6.267578	5.985754	2.595007	4.947183
25	H	5.956364	6.576300	6.421925	2.784413	5.120372
26	H	5.940947	7.232949	6.773931	3.610181	5.964532
27	H	5.927144	6.013278	6.100570	2.039159	4.406399
		21	22	23	24	25
21	H	0.000000				
22	H	2.501875	0.000000			
23	H	4.289488	2.430230	0.000000		
24	C	6.284825	4.970004	2.622509	0.000000	
25	H	6.697682	5.276482	2.943085	1.099525	0.000000
26	H	5.992932	4.366841	1.983014	1.092021	1.766734
27	H	7.201344	5.936511	3.595212	1.093094	1.766571
		26	27			
26	H	0.000000				
27	H	1.750322	0.000000			

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.658797	-0.995723	0.019695
2	6	0	-2.460425	-1.660510	-0.010017
3	6	0	-1.217590	-0.950786	-0.018178
4	6	0	-1.225197	0.496793	-0.009593
5	6	0	-2.505134	1.144732	0.027744
6	6	0	-3.676616	0.428183	0.043944
7	6	0	0.002646	-1.632806	-0.031098
8	6	0	-0.001023	1.211627	-0.029533
9	6	0	1.226378	0.501142	-0.010136
10	6	0	1.220944	-0.947359	-0.019247
11	6	0	2.464488	-1.656094	-0.011917
12	1	0	2.437069	-2.743445	-0.025978
13	6	0	3.662354	-0.990950	0.018626
14	6	0	3.678822	0.432855	0.045041
15	6	0	2.507080	1.148731	0.029317
16	1	0	0.004231	-2.721166	-0.042021
17	1	0	-4.594244	-1.548982	0.028192
18	1	0	-2.432417	-2.747866	-0.023012
19	1	0	-2.556363	2.227251	0.057941
20	1	0	-4.628415	0.952157	0.077483
21	1	0	4.598183	-1.543556	0.026894
22	1	0	4.630168	0.957548	0.080176
23	1	0	2.560200	2.230708	0.062476
24	6	0	-0.012339	2.726759	-0.053842
25	1	0	-0.088309	3.149895	0.958157
26	1	0	0.891187	3.134359	-0.512114
27	1	0	-0.854829	3.113536	-0.633038

```
 Rotational constants (GHZ):      1.3930877      0.4478557
0.3397073
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8443141582 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860567720     A.U. after   10 cycles
             Convg  =    0.4136D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000350416   -0.000177884   -0.000024780
      2        6          -0.000353946    0.000008464    0.000081499
      3        6          -0.000351026    0.000262271    0.000014679
      4        6           0.000276507   -0.000140342   -0.000150576
      5        6          -0.000080057   -0.000211190    0.000180346
      6        6           0.000114975    0.000295643   -0.000025411
      7        6           0.000073005   -0.000016024   -0.000016955
      8        6           0.000226192    0.000341032   -0.000090820
      9        6          -0.000334930   -0.000156544   -0.000029512
     10        6          -0.000156203    0.000285484    0.000000557
     11        6           0.000212708    0.000330913    0.000066201
     12        1          -0.000071002   -0.000151948   -0.000007693
     13        6           0.000034122   -0.000451144   -0.000009866
```

```
     14        6          -0.000397412    0.000058231   -0.000042134
     15        6           0.000276694   -0.000199141    0.000131361
     16        1           0.000052732   -0.000066464   -0.000003128
     17        1          -0.000122875    0.000002201    0.000013919
     18        1           0.000148830   -0.000024356   -0.000016828
     19        1          -0.000058640    0.000008778    0.000019929
     20        1          -0.000086043   -0.000052990   -0.000011709
     21        1           0.000058039    0.000105592    0.000000457
     22        1           0.000061535    0.000059900   -0.000005232
     23        1          -0.000021999    0.000141782   -0.000008223
     24        6           0.000427088   -0.000344997   -0.000060764
     25        1           0.000012908   -0.000022958   -0.000089948
     26        1          -0.000298801   -0.000008810    0.000125152
     27        1           0.000007184    0.000124499   -0.000040522
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000451144 RMS     0.000173387


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000322038 RMS     0.000090538
 Search for a local minimum.
 Step number  19 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
 DE= -1.98D-06 DEPred=-1.29D-06 R= 1.53D+00
 SS=  1.41D+00  RLast= 1.99D-02 DXNew= 8.4090D-02 5.9795D-02
 Trust test= 1.53D+00 RLast= 1.99D-02 DXMaxT set to 5.98D-02
     Eigenvalues ---   -0.17235   0.00000   0.01218   0.01580
0.01774
     Eigenvalues ---    0.01785   0.01817   0.01821   0.01866
0.01975
     Eigenvalues ---    0.01979   0.01993   0.02055   0.02075
0.02105
     Eigenvalues ---    0.02117   0.02143   0.02158   0.02221
0.02233
     Eigenvalues ---    0.02300   0.02354   0.02758   0.06656
0.06831
     Eigenvalues ---    0.12403   0.15667   0.15951   0.15998
0.15999
     Eigenvalues ---    0.16000   0.16000   0.16016   0.16033
0.16112
```

```
     Eigenvalues ---    0.16421   0.19876   0.22001   0.22117
0.22469
     Eigenvalues ---    0.22705   0.23428   0.24456   0.24552
0.24982
     Eigenvalues ---    0.27118   0.27675   0.30404   0.33541
0.33617
     Eigenvalues ---    0.33631   0.33681   0.33682   0.33694
0.33805
     Eigenvalues ---    0.33895   0.34131   0.36207   0.36868
0.37250
     Eigenvalues ---    0.37698   0.38592   0.38767   0.39585
0.40239
     Eigenvalues ---    0.41100   0.41821   0.43962   0.44970
0.45672
     Eigenvalues ---    0.49432   0.49842   0.50047   0.51294
0.55287
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is  -1.72D-01 should be greater than     0.000000
Eigenvector:
                          R15       A23       A24       A2        A35
   1                    0.23447  -0.21984   0.21372  -0.20009  -
0.19783
                          A45       A12       A33       R22       R17
```

```
   1                 -0.19367  -0.18311  -0.17790  -0.17701
0.17685
 Eigenvalue     2 is   4.01D-06 Eigenvector:
                          D44       D46       D41       D45       D43
   1                   0.43410   0.40960   0.40899   0.40798
0.38448
                          D42       A23       A24       A45       D27
   1                   0.38287   0.04617  -0.04534   0.03710  -
0.02704
 Use linear search instead of GDIIS.
 RFO step:  Lambda=-8.16971370D-06 EMin= 1.72345718D-01
 Quartic linear search produced a step of  0.60613.
 Maximum step size (   0.060) exceeded in Quadratic search.
    -- Step size scaled by   0.406
 Iteration  1 RMS(Cart)=  0.00593412 RMS(Int)=  0.00005284
 Iteration  2 RMS(Cart)=  0.00005473 RMS(Int)=  0.00000024
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000024
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.59032  -0.00022  -0.00005   0.00018   0.00013
2.59045
    R2        2.69139   0.00011   0.00005  -0.00021  -0.00016
2.69123
    R3        2.05383   0.00006  -0.00004   0.00005   0.00001
2.05384
    R4        2.70463   0.00005   0.00006  -0.00025  -0.00019
2.70444
    R5        2.05563   0.00010  -0.00006   0.00006   0.00000
2.05563
    R6        2.73561  -0.00028  -0.00004  -0.00033  -0.00037
2.73524
    R7        2.64176   0.00006   0.00004   0.00005   0.00009
2.64185
    R8        2.71191   0.00011   0.00010  -0.00035  -0.00025
2.71166
    R9        2.67914   0.00011   0.00015   0.00004   0.00019
2.67933
   R10        2.59525  -0.00012  -0.00002   0.00020   0.00018
2.59543
   R11        2.04875   0.00004  -0.00007   0.00012   0.00005
2.04879
   R12        2.05416   0.00009  -0.00005   0.00004  -0.00002
2.05414
   R13        2.64172   0.00001  -0.00002  -0.00006  -0.00008
2.64164
   R14        2.05681   0.00008  -0.00006   0.00006   0.00000
2.05680
   R15        2.68027  -0.00027  -0.00014   0.00001  -0.00013
2.68014
   R16        2.86363  -0.00029  -0.00013  -0.00009  -0.00022
2.86341
```

This journal is © The Royal Society of Chemistry 2014

R17	2.73734	-0.00017	-0.00005	0.00051	0.00046
2.73780					
R18	2.71301	0.00000	0.00000	-0.00002	-0.00002
2.71299					
R19	2.70486	0.00008	0.00008	-0.00011	-0.00002
2.70483					
R20	2.05562	0.00010	-0.00006	0.00005	-0.00001
2.05561					
R21	2.58984	-0.00023	-0.00004	-0.00002	-0.00006
2.58978					
R22	2.69124	0.00018	0.00011	-0.00019	-0.00008
2.69116					
R23	2.05383	0.00006	-0.00004	0.00004	0.00000
2.05383					
R24	2.59499	-0.00018	-0.00005	0.00003	-0.00002
2.59497					
R25	2.05416	0.00008	-0.00006	0.00003	-0.00002
2.05413					
R26	2.04806	0.00014	0.00002	-0.00005	-0.00003
2.04803					
R27	2.07780	-0.00009	0.00007	-0.00007	-0.00001
2.07779					
R28	2.06362	-0.00022	-0.00001	-0.00052	-0.00053
2.06309					
R29	2.06565	0.00000	0.00003	0.00054	0.00056
2.06621					
A1	2.08999	-0.00010	-0.00001	0.00023	0.00022
2.09021					
A2	2.10106	0.00016	0.00008	-0.00062	-0.00054
2.10052					
A3	2.09213	-0.00006	-0.00007	0.00039	0.00032
2.09245					
A4	2.11625	0.00000	-0.00004	-0.00003	-0.00007
2.11617					
A5	2.10314	0.00012	0.00010	-0.00048	-0.00038
2.10276					
A6	2.06378	-0.00012	-0.00006	0.00051	0.00045
2.06424					
A7	2.08435	0.00016	0.00008	-0.00028	-0.00020
2.08414					
A8	2.11309	-0.00010	-0.00009	0.00067	0.00058
2.11367					
A9	2.08575	-0.00006	0.00001	-0.00039	-0.00038
2.08537					
A10	2.04466	-0.00014	-0.00006	0.00052	0.00046
2.04512					
A11	2.09390	0.00006	-0.00005	0.00051	0.00046
2.09436					
A12	2.14461	0.00009	0.00010	-0.00102	-0.00092
2.14368					
A13	2.12413	0.00003	-0.00003	-0.00018	-0.00021
2.12393					

This journal is © The Royal Society of Chemistry 2014

A14	2.08712	0.00003	0.00004	-0.00031	-0.00027
2.08685					
A15	2.07183	-0.00006	-0.00001	0.00049	0.00048
2.07231					
A16	2.10687	0.00005	0.00005	-0.00025	-0.00020
2.10667					
A17	2.08679	-0.00008	-0.00007	0.00038	0.00031
2.08711					
A18	2.08952	0.00003	0.00002	-0.00014	-0.00011
2.08940					
A19	2.11930	-0.00003	-0.00004	0.00008	0.00004
2.11934					
A20	2.08198	0.00003	0.00003	0.00000	0.00003
2.08201					
A21	2.08188	0.00000	0.00000	-0.00007	-0.00007
2.08180					
A22	2.08802	-0.00001	-0.00003	0.00002	-0.00001
2.08800					
A23	2.09198	-0.00012	0.00015	-0.00258	-0.00243
2.08955					
A24	2.10311	0.00013	-0.00014	0.00258	0.00244
2.10556					
A25	2.09161	0.00002	0.00003	-0.00052	-0.00048
2.09112					
A26	2.14885	0.00011	-0.00008	0.00083	0.00074
2.14959					
A27	2.04270	-0.00012	0.00005	-0.00031	-0.00026
2.04243					
A28	2.08706	0.00003	0.00001	0.00031	0.00032
2.08738					
A29	2.11111	-0.00016	-0.00003	-0.00027	-0.00030
2.11082					
A30	2.08501	0.00013	0.00002	-0.00004	-0.00002
2.08498					
A31	2.06348	-0.00014	-0.00008	0.00034	0.00026
2.06373					
A32	2.11667	0.00000	-0.00004	0.00016	0.00012
2.11678					
A33	2.10303	0.00014	0.00013	-0.00050	-0.00038
2.10265					
A34	2.08948	-0.00012	-0.00001	-0.00004	-0.00005
2.08943					
A35	2.10134	0.00017	0.00008	-0.00047	-0.00039
2.10095					
A36	2.09236	-0.00005	-0.00007	0.00051	0.00044
2.09279					
A37	2.10727	0.00008	0.00005	-0.00005	0.00000
2.10727					
A38	2.08667	-0.00006	-0.00003	0.00035	0.00032
2.08699					
A39	2.08924	-0.00002	-0.00001	-0.00031	-0.00032
2.08892					

A40	2.12510	0.00004	-0.00006	0.00027	0.00021	2.12530
A41	2.08850	0.00003	-0.00005	0.00035	0.00029	2.08879
A42	2.06948	-0.00007	0.00012	-0.00062	-0.00051	2.06898
A43	1.95037	-0.00007	0.00004	0.00048	0.00052	1.95089
A44	1.95384	0.00032	-0.00010	0.00142	0.00132	1.95516
A45	1.94769	0.00010	-0.00016	-0.00187	-0.00202	1.94567
A46	1.87525	-0.00013	0.00004	0.00027	0.00031	1.87556
A47	1.87367	-0.00004	0.00013	-0.00055	-0.00042	1.87325
A48	1.85800	-0.00020	0.00006	0.00023	0.00029	1.85829
D1	-0.00074	-0.00002	-0.00026	0.00024	-0.00002	-0.00076
D2	3.13546	-0.00001	-0.00032	0.00023	-0.00009	3.13537
D3	-3.13875	0.00000	0.00001	-0.00024	-0.00023	-3.13898
D4	-0.00255	0.00000	-0.00005	-0.00025	-0.00030	-0.00285
D5	0.00860	0.00001	0.00022	-0.00020	0.00002	0.00862
D6	-3.13101	0.00001	0.00048	-0.00021	0.00028	-3.13073
D7	-3.13655	-0.00001	-0.00005	0.00027	0.00023	-3.13632
D8	0.00702	-0.00001	0.00021	0.00027	0.00048	0.00750
D9	-0.01187	0.00000	-0.00028	0.00033	0.00005	-0.01182
D10	3.12705	-0.00002	-0.00075	0.00075	0.00000	3.12705
D11	3.13499	-0.00001	-0.00022	0.00035	0.00013	3.13512
D12	-0.00927	-0.00003	-0.00069	0.00076	0.00007	-0.00920
D13	0.01631	0.00004	0.00084	-0.00091	-0.00008	0.01623
D14	-3.13183	-0.00002	-0.00024	0.00037	0.00012	-3.13170
D15	-3.12266	0.00006	0.00129	-0.00132	-0.00003	-3.12268
D16	0.01239	0.00000	0.00022	-0.00004	0.00017	0.01257
D17	-3.12492	0.00005	0.00134	-0.00054	0.00080	-3.12412

This journal is © The Royal Society of Chemistry 2014

D18	0.00741	0.00001	0.00071	0.00004	0.00075	0.00816
D19	0.01400	0.00003	0.00087	-0.00012	0.00075	0.01475
D20	-3.13685	-0.00001	0.00025	0.00045	0.00070	-3.13615
D21	-0.00889	-0.00005	-0.00089	0.00097	0.00008	-0.00881
D22	3.11765	-0.00004	-0.00073	0.00097	0.00024	3.11789
D23	3.13946	0.00001	0.00022	-0.00035	-0.00013	3.13932
D24	-0.01720	0.00003	0.00039	-0.00035	0.00003	-0.01716
D25	-0.03870	-0.00003	-0.00133	0.00000	-0.00133	-0.04002
D26	3.11621	0.00002	0.00020	-0.00188	-0.00168	3.11453
D27	3.09596	-0.00010	-0.00247	0.00136	-0.00111	3.09485
D28	-0.03232	-0.00004	-0.00095	-0.00052	-0.00146	-0.03378
D29	-0.00352	0.00003	0.00038	-0.00043	-0.00005	-0.00357
D30	3.13609	0.00003	0.00012	-0.00042	-0.00031	3.13578
D31	-3.13018	0.00002	0.00021	-0.00042	-0.00021	-3.13039
D32	0.00943	0.00001	-0.00005	-0.00042	-0.00047	0.00896
D33	-0.01359	-0.00003	-0.00083	0.00032	-0.00051	-0.01410
D34	3.12469	-0.00004	-0.00117	0.00031	-0.00086	3.12383
D35	3.13726	0.00001	-0.00020	-0.00026	-0.00046	3.13680
D36	-0.00764	-0.00001	-0.00055	-0.00027	-0.00081	-0.00845
D37	0.03906	0.00004	0.00137	0.00018	0.00155	0.04061
D38	-3.09373	0.00006	0.00180	0.00041	0.00220	-3.09153
D39	-3.11593	-0.00002	-0.00016	0.00203	0.00187	-3.11406
D40	0.03446	0.00000	0.00027	0.00225	0.00252	0.03698
D41	1.49244	-0.00007	0.00363	-0.02437	-0.02074	1.47169
D42	-2.68627	-0.00006	0.00364	-0.02269	-0.01905	-2.70532
D43	-0.60573	-0.00003	0.00355	-0.02271	-0.01916	-0.62489

This journal is © The Royal Society of Chemistry 2014

D44	-1.63573	-0.00001	0.00517	-0.02624	-0.02108	-1.65680
D45	0.46876	0.00000	0.00518	-0.02456	-0.01938	0.44937
D46	2.54929	0.00003	0.00508	-0.02458	-0.01950	2.52979
D47	-0.01320	-0.00001	-0.00031	-0.00035	-0.00066	-0.01385
D48	3.13165	0.00001	0.00003	-0.00034	-0.00031	3.13134
D49	3.12012	-0.00003	-0.00071	-0.00056	-0.00127	3.11886
D50	-0.01821	-0.00001	-0.00037	-0.00055	-0.00092	-0.01913
D51	-3.13965	0.00001	0.00010	0.00005	0.00015	-3.13949
D52	0.01797	-0.00002	-0.00024	0.00073	0.00049	0.01846
D53	0.01051	0.00003	0.00052	0.00027	0.00079	0.01131
D54	-3.11506	0.00000	0.00018	0.00095	0.00113	-3.11393
D55	0.01061	0.00002	0.00038	0.00016	0.00054	0.01115
D56	-3.12544	0.00000	0.00037	0.00042	0.00079	-3.12465
D57	-3.13429	0.00000	0.00004	0.00016	0.00019	-3.13410
D58	0.01285	-0.00001	0.00003	0.00041	0.00044	0.01329
D59	0.00109	0.00002	0.00019	0.00004	0.00022	0.00131
D60	3.13830	0.00001	0.00015	-0.00005	0.00010	3.13840
D61	-3.13483	0.00000	0.00018	0.00029	0.00048	-3.13436
D62	0.00238	0.00000	0.00014	0.00021	0.00035	0.00273
D63	-0.00928	0.00000	-0.00005	-0.00033	-0.00038	-0.00966
D64	3.13002	0.00000	-0.00029	-0.00056	-0.00086	3.12917
D65	3.13667	0.00001	-0.00001	-0.00024	-0.00025	3.13642
D66	-0.00721	0.00000	-0.00025	-0.00048	-0.00073	-0.00794
D67	0.00316	-0.00003	-0.00032	0.00016	-0.00016	0.00300
D68	3.12890	0.00000	0.00002	-0.00050	-0.00048	3.12842
D69	-3.13614	-0.00002	-0.00007	0.00040	0.00032	-3.13582

```
   D70       -0.01040   0.00001   0.00026  -0.00026   0.00000  -
0.01040
         Item               Value     Threshold  Converged?
 Maximum Force            0.000322     0.000450     YES
 RMS     Force            0.000091     0.000300     YES
 Maximum Displacement     0.041678     0.001800     NO
 RMS     Displacement     0.005935     0.001200     NO
 Predicted change in Energy=-3.616028D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792854   -5.428220    0.009615
      2          6           0       -3.422686   -5.396684   -0.017884
      3          6           0       -2.708729   -4.156418   -0.029185
      4          6           0       -3.446800   -2.911313   -0.026155
      5          6           0       -4.878679   -2.998288    0.009015
      6          6           0       -5.527785   -4.208507    0.028364
      7          6           0       -1.311055   -4.127740   -0.039834
      8          6           0       -2.752233   -1.675469   -0.049391
      9          6           0       -1.334178   -1.667465   -0.026198
     10          6           0       -0.606657   -2.920327   -0.030063
     11          6           0        0.824539   -2.903339   -0.019322
     12          1           0        1.350722   -3.855335   -0.029639
     13          6           0        1.522015   -1.724015    0.010136
     14          6           0        0.816648   -0.487068    0.032227
     15          6           0       -0.556179   -0.461527    0.012957
     16          1           0       -0.759246   -5.065874   -0.047248
     17          1           0       -5.320200   -6.378496    0.020328
     18          1           0       -2.849565   -6.321209   -0.026585
     19          1           0       -5.469384   -2.089531    0.034823
     20          1           0       -6.613944   -4.236893    0.060419
     21          1           0        2.608792   -1.728379    0.020926
     22          1           0        1.372010    0.446693    0.067318
     23          1           0       -1.056727    0.499247    0.043350
     24          6           0       -3.531378   -0.376285   -0.081678
     25          1           0       -3.833070   -0.056395    0.926091
     26          1           0       -2.952941    0.437075   -0.524120
     27          1           0       -4.441864   -0.470250   -0.679750
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                      1          2          3          4          5
    1  C    0.000000
    2  C    1.370807   0.000000
    3  C    2.441835   1.431126   0.000000
    4  C    2.854463   2.485501   1.447426   0.000000
    5  C    2.431447   2.805876   2.459961   1.434950   0.000000
```

This journal is © The Royal Society of Chemistry 2014

6	C	1.424139	2.417714	2.820124	2.452791	1.373442
7	C	3.717071	2.463673	1.398009	2.457903	3.742458
8	C	4.272090	3.781262	2.481413	1.417842	2.505003
9	C	5.109501	4.274226	2.843288	2.451598	3.786268
10	C	4.880097	3.750001	2.438571	2.840160	4.272912
11	C	6.158811	4.925006	3.748905	4.271351	5.704079
12	H	6.341847	5.016105	4.070601	4.889520	6.288200
13	C	7.321113	6.159492	4.880300	5.108827	6.526305
14	C	7.475426	6.486816	5.088829	4.904830	6.224429
15	C	6.528205	5.707327	4.276385	3.789284	5.011904
16	H	4.050249	2.684065	2.151260	3.444637	4.609534
17	H	1.086846	2.136815	3.429266	3.941211	3.408941
18	H	2.138952	1.087792	2.169369	3.461803	3.893633
19	H	3.406636	3.889602	3.449251	2.184008	1.084176
20	H	2.176743	3.396377	3.907071	3.434452	2.132587
21	H	8.274860	7.059510	5.845846	6.170230	7.594408
22	H	8.516072	7.559194	6.152266	5.874170	7.137395
23	H	7.006757	6.353228	4.940606	4.165237	5.180854
24	C	5.207849	5.021980	3.868968	2.537046	2.949296
25	H	5.533318	5.438583	4.357394	3.034227	3.254084
26	H	6.170238	5.874493	4.626530	3.421048	3.974220
27	H	5.017955	5.074104	4.124903	2.715903	2.656347

		6	7	8	9	10
6	C	0.000000				
7	C	4.218054	0.000000			
8	C	3.758460	2.844419	0.000000		
9	C	4.903694	2.460422	1.418267	0.000000	
10	C	5.087270	1.397898	2.480634	1.448781	0.000000
11	C	6.485195	2.461776	3.781781	2.487466	1.431337
12	H	6.887811	2.675699	4.646122	3.463448	2.169233
13	C	7.474805	3.715734	4.274938	2.856983	2.442135
14	C	7.355335	4.217441	3.762428	2.454139	2.819650
15	C	6.225509	3.743493	2.510019	1.435653	2.459694
16	H	4.845591	1.088413	3.932792	3.446763	2.151035
17	H	2.179910	4.598126	5.358898	6.171253	5.846278
18	H	3.411655	2.679271	4.646816	4.894256	4.073898
19	H	2.119791	4.631583	2.749809	4.157138	4.933614
20	H	1.087003	5.304959	4.635274	5.872427	6.150531
21	H	8.506172	4.596284	5.361747	3.943722	3.429643
22	H	8.323435	5.304315	4.639674	3.435384	3.906589
23	H	6.492575	4.634718	2.759117	2.185510	3.449846
24	C	4.322462	4.359472	1.515252	2.549100	3.876701
25	H	4.573621	4.885634	2.177424	3.121997	4.418832
26	H	5.340084	4.875229	2.174509	2.701371	4.125687
27	H	3.956667	4.856819	2.169045	3.393843	4.597150

		11	12	13	14	15
11	C	0.000000				
12	H	1.087783	0.000000			
13	C	1.370455	2.138563	0.000000		
14	C	2.416834	3.410907	1.424103	0.000000	
15	C	2.805328	3.893073	2.431619	1.373199	0.000000
16	H	2.680618	2.432628	4.046661	4.843059	4.609216

This journal is © The Royal Society of Chemistry 2014

17	H	7.059469	7.132323	8.275277	8.507054	7.596478
18	H	5.018060	4.870621	6.343994	6.890703	6.292619
19	H	6.346548	7.045286	7.000991	6.487071	5.175950
20	H	7.557496	7.974308	8.515334	8.323201	7.138078
21	H	2.136752	2.471688	1.086839	2.180083	3.409108
22	H	3.395578	4.303174	2.176636	1.087000	2.132072
23	H	3.888532	4.976296	3.404982	2.117185	1.083771
24	C	5.036259	5.995114	5.230830	4.350928	2.977924
25	H	5.540055	6.497466	5.683033	4.754403	3.425779
26	H	5.067794	6.098427	4.998096	3.920887	2.615417
27	H	5.838757	6.740586	6.133166	5.306519	3.946957

		16	17	18	19	20
16	H	0.000000				
17	H	4.746561	0.000000			
18	H	2.438386	2.471745	0.000000		
19	H	5.572320	4.291583	4.977381	0.000000	
20	H	5.914075	2.502368	4.303777	2.433482	0.000000
21	H	4.742067	9.191980	7.133723	8.086257	9.557879
22	H	5.911326	9.558823	7.977156	7.296449	9.258050
23	H	5.573803	8.092038	7.052502	5.115993	7.301642
24	C	5.447765	6.263931	5.984148	2.589334	4.942337
25	H	5.957404	6.557509	6.412704	2.757812	5.095018
26	H	5.943244	7.235492	6.777362	3.609521	5.965786
27	H	5.922963	6.014063	6.098833	2.046578	4.410598

		21	22	23	24	25
21	H	0.000000				
22	H	2.502543	0.000000			
23	H	4.289388	2.429424	0.000000		
24	C	6.288114	4.974204	2.627943	0.000000	
25	H	6.716579	5.299381	2.965814	1.099521	0.000000
26	H	5.993257	4.365213	1.980281	1.091742	1.766706
27	H	7.196220	5.932961	3.594712	1.093391	1.766531

		26	27
26	H	0.000000	
27	H	1.750529	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.658074	-0.996454	0.020702
2	6	0	-2.459680	-1.661304	-0.009912
3	6	0	-1.216969	-0.951576	-0.018652
4	6	0	-1.224925	0.495800	-0.009629
5	6	0	-2.504582	1.143949	0.028612
6	6	0	-3.676144	0.427357	0.045350

```
      7          6           0        0.003725   -1.632857   -0.032492
      8          6           0       -0.001184    1.211557   -0.030274
      9          6           0        1.226665    0.501998   -0.010389
     10          6           0        1.221597   -0.946741   -0.020249
     11          6           0        2.465322   -1.655133   -0.012817
     12          1           0        2.438488   -2.742484   -0.027627
     13          6           0        3.663036   -0.989841    0.019032
     14          6           0        3.679187    0.433895    0.047011
     15          6           0        2.507319    1.149538    0.031058
     16          1           0        0.006011   -2.721203   -0.044411
     17          1           0       -4.593241   -1.550189    0.029406
     18          1           0       -2.432127   -2.748666   -0.023122
     19          1           0       -2.555270    2.226515    0.058916
     20          1           0       -4.627843    0.951431    0.079863
     21          1           0        4.598736   -1.542668    0.027250
     22          1           0        4.630203    0.959034    0.083987
     23          1           0        2.560716    2.231431    0.065913
     24          6           0       -0.017280    2.726499   -0.056286
     25          1           0       -0.115735    3.150803    0.953278
     26          1           0        0.892680    3.138051   -0.497304
     27          1           0       -0.850691    3.107840   -0.652532
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3931530      0.4478611
0.3397211
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8552314578 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860571037     A.U. after   10 cycles
             Convg  =    0.6625D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000381581   -0.000241040   -0.000040371
      2        6          -0.000384015   -0.000020068    0.000076470
      3        6          -0.000337136    0.000301907    0.000034334
      4        6           0.000317402   -0.000084882   -0.000185856
      5        6          -0.000102383   -0.000283241    0.000154492
      6        6           0.000119493    0.000384121   -0.000004425
      7        6           0.000073488   -0.000039401   -0.000032361
```

```
      8        6           0.000188969    0.000226771   -0.000008104
      9        6          -0.000346990   -0.000224016    0.000000862
     10        6          -0.000182017    0.000299792    0.000014550
     11        6           0.000255079    0.000353457    0.000058425
     12        1          -0.000104520   -0.000173809   -0.000011911
     13        6           0.000058145   -0.000502934   -0.000025875
     14        6          -0.000443216    0.000085360   -0.000021568
     15        6           0.000286875   -0.000147396    0.000081540
     16        1           0.000053999   -0.000068363    0.000012724
     17        1          -0.000162973    0.000023888    0.000027376
     18        1           0.000182665   -0.000005701   -0.000023069
     19        1          -0.000075894   -0.000019467    0.000030385
     20        1          -0.000091670   -0.000081562   -0.000022648
     21        1           0.000058000    0.000151640    0.000011427
     22        1           0.000091119    0.000050572   -0.000014827
     23        1          -0.000077188    0.000141486   -0.000033730
     24        6           0.000351190   -0.000354395   -0.000076449
     25        1           0.000040569   -0.000033720   -0.000084734
     26        1          -0.000215655    0.000053519    0.000111537
     27        1           0.000065081    0.000207481   -0.000028195
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000502934 RMS     0.000182946


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000352782 RMS     0.000100193
 Search for a local minimum.
 Step number  20 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
20
 DE= -3.32D-06 DEPred=-3.62D-06 R= 9.17D-01
 SS=  1.41D+00  RLast= 4.92D-02 DXNew= 1.0056D-01 1.4770D-01
 Trust test= 9.17D-01 RLast= 4.92D-02 DXMaxT set to 1.01D-01
 Use linear search instead of GDIIS.
     Eigenvalues ---   -0.27299  -0.07983   0.00000   0.01490
0.01718
     Eigenvalues ---    0.01770   0.01815   0.01819   0.01871
0.01923
     Eigenvalues ---    0.01976   0.01988   0.02021   0.02063
0.02089
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02115   0.02144   0.02159   0.02187
0.02215
     Eigenvalues ---    0.02237   0.02354   0.02375   0.03097
0.06793
     Eigenvalues ---    0.06808   0.14200   0.15754   0.15975
0.15996
     Eigenvalues ---    0.16000   0.16000   0.16003   0.16008
0.16088
     Eigenvalues ---    0.16197   0.18124   0.21749   0.21932
0.22000
     Eigenvalues ---    0.22652   0.23333   0.23790   0.24450
0.24973
     Eigenvalues ---    0.25414   0.27287   0.29924   0.32852
0.33541
     Eigenvalues ---    0.33612   0.33631   0.33639   0.33682
0.33683
     Eigenvalues ---    0.33724   0.34205   0.34879   0.35799
0.37140
     Eigenvalues ---    0.37250   0.38137   0.38425   0.39282
0.40228
     Eigenvalues ---    0.41119   0.41646   0.42236   0.44610
0.45381
     Eigenvalues ---    0.46186   0.49294   0.49851   0.49986
0.51296
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---  1000.000001000.00000
 RFO step:  Lambda=-2.73002441D-01 EMin=-2.72992040D-01
 RFO eigenvector is Hessian eigenvector with negative curvature.
 Taking step of  2.51D-01 in eigenvector direction.  Step.Grad= -
4.24D-04.
 Quartic linear search produced a step of  2.00000.
 Maximum step size (   0.101) exceeded in Quadratic search.
    -- Step size scaled by   0.400
 Iteration  1 RMS(Cart)=  0.02066604 RMS(Int)=  0.00040098
 Iteration  2 RMS(Cart)=  0.00044234 RMS(Int)=  0.00004919
 Iteration  3 RMS(Cart)=  0.00000013 RMS(Int)=  0.00004919
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.59045  -0.00022   0.00026  -0.00908  -0.00881
2.58164
    R2        2.69123   0.00013  -0.00032   0.00580   0.00547
2.69670
    R3        2.05384   0.00006   0.00001   0.00352   0.00353
2.05737
    R4        2.70444   0.00007  -0.00039   0.00188   0.00151
2.70595
    R5        2.05563   0.00010  -0.00001   0.00693   0.00692
2.06255
    R6        2.73524  -0.00023  -0.00075  -0.01092  -0.01167
2.72357
    R7        2.64185   0.00007   0.00018   0.00390   0.00407
2.64593
    R8        2.71166   0.00016  -0.00049   0.00474   0.00424
2.71590
    R9        2.67933   0.00014   0.00038   0.00215   0.00253
2.68186
   R10        2.59543  -0.00014   0.00037  -0.00657  -0.00621
2.58922
   R11        2.04879   0.00003   0.00009   0.00301   0.00310
2.05190
   R12        2.05414   0.00009  -0.00004   0.00715   0.00711
2.06125
   R13        2.64164   0.00000  -0.00015   0.00037   0.00022
2.64186
   R14        2.05680   0.00009  -0.00001   0.00594   0.00593
2.06274
   R15        2.68014  -0.00035  -0.00027  -0.01983  -0.02009
2.66005
   R16        2.86341  -0.00023  -0.00044  -0.02929  -0.02973
2.83368
   R17        2.73780  -0.00023   0.00091  -0.01505  -0.01413
2.72367
   R18        2.71299   0.00000  -0.00003  -0.00399  -0.00403
2.70896
   R19        2.70483   0.00010  -0.00005   0.00284   0.00281
2.70764
```

This journal is © The Royal Society of Chemistry 2014

R20	2.05561	0.00010	-0.00002	0.00692	0.00690
2.06251					
R21	2.58978	-0.00020	-0.00012	-0.00716	-0.00727
2.58252					
R22	2.69116	0.00021	-0.00016	0.00963	0.00947
2.70063					
R23	2.05383	0.00006	0.00000	0.00344	0.00344
2.05727					
R24	2.59497	-0.00019	-0.00004	-0.00754	-0.00759
2.58738					
R25	2.05413	0.00009	-0.00005	0.00708	0.00703
2.06116					
R26	2.04803	0.00016	-0.00007	0.01019	0.01013
2.05816					
R27	2.07779	-0.00010	-0.00002	-0.00137	-0.00139
2.07641					
R28	2.06309	-0.00012	-0.00106	0.00127	0.00022
2.06331					
R29	2.06621	-0.00006	0.00112	-0.00152	-0.00040
2.06581					
A1	2.09021	-0.00012	0.00044	-0.01159	-0.01116
2.07905					
A2	2.10052	0.00022	-0.00108	0.01868	0.01761
2.11813					
A3	2.09245	-0.00010	0.00064	-0.00709	-0.00645
2.08600					
A4	2.11617	0.00001	-0.00014	0.00226	0.00213
2.11831					
A5	2.10276	0.00015	-0.00076	0.01335	0.01258
2.11534					
A6	2.06424	-0.00016	0.00091	-0.01560	-0.01471
2.04953					
A7	2.08414	0.00018	-0.00041	0.01269	0.01230
2.09644					
A8	2.11367	-0.00016	0.00116	-0.01167	-0.01051
2.10316					
A9	2.08537	-0.00002	-0.00075	-0.00102	-0.00179
2.08358					
A10	2.04512	-0.00020	0.00093	-0.01536	-0.01443
2.03070					
A11	2.09436	-0.00001	0.00092	0.00104	0.00195
2.09631					
A12	2.14368	0.00021	-0.00185	0.01429	0.01244
2.15613					
A13	2.12393	0.00005	-0.00041	0.00591	0.00547
2.12940					
A14	2.08685	0.00005	-0.00054	0.00763	0.00710
2.09395					
A15	2.07231	-0.00010	0.00096	-0.01352	-0.01256
2.05975					
A16	2.10667	0.00007	-0.00040	0.00606	0.00564
2.11232					

A17	2.08711	-0.00012	0.00062	-0.00687	-0.00624
2.08087					
A18	2.08940	0.00005	-0.00023	0.00081	0.00059
2.08999					
A19	2.11934	-0.00005	0.00008	-0.00307	-0.00300
2.11634					
A20	2.08201	0.00004	0.00006	0.00231	0.00237
2.08438					
A21	2.08180	0.00001	-0.00014	0.00075	0.00061
2.08241					
A22	2.08800	-0.00001	-0.00003	-0.00412	-0.00414
2.08386					
A23	2.08955	0.00019	-0.00485	0.02212	0.01726
2.10682					
A24	2.10556	-0.00017	0.00489	-0.01804	-0.01316
2.09240					
A25	2.09112	0.00010	-0.00097	0.01065	0.00970
2.10082					
A26	2.14959	-0.00002	0.00149	-0.00512	-0.00364
2.14596					
A27	2.04243	-0.00007	-0.00053	-0.00552	-0.00606
2.03637					
A28	2.08738	0.00000	0.00063	-0.00337	-0.00273
2.08465					
A29	2.11082	-0.00011	-0.00059	-0.00446	-0.00506
2.10575					
A30	2.08498	0.00011	-0.00005	0.00783	0.00779
2.09278					
A31	2.06373	-0.00018	0.00051	-0.01621	-0.01571
2.04803					
A32	2.11678	-0.00001	0.00023	0.00103	0.00129
2.11807					
A33	2.10265	0.00018	-0.00075	0.01519	0.01443
2.11708					
A34	2.08943	-0.00012	-0.00010	-0.01061	-0.01070
2.07874					
A35	2.10095	0.00022	-0.00078	0.01817	0.01739
2.11834					
A36	2.09279	-0.00010	0.00087	-0.00756	-0.00669
2.08610					
A37	2.10727	0.00007	0.00000	0.00507	0.00506
2.11233					
A38	2.08699	-0.00009	0.00064	-0.00486	-0.00422
2.08277					
A39	2.08892	0.00002	-0.00064	-0.00021	-0.00084
2.08808					
A40	2.12530	0.00001	0.00041	0.00222	0.00262
2.12792					
A41	2.08879	-0.00001	0.00059	0.00156	0.00216
2.09095					
A42	2.06898	0.00000	-0.00101	-0.00374	-0.00474
2.06423					

This journal is © The Royal Society of Chemistry 2014

A43	1.95089	-0.00012	0.00104	-0.00026	0.00075	1.95164
A44	1.95516	0.00026	0.00264	0.02535	0.02776	1.98292
A45	1.94567	0.00022	-0.00405	0.03184	0.02755	1.97322
A46	1.87556	-0.00012	0.00062	-0.02008	-0.01948	1.85609
A47	1.87325	-0.00004	-0.00085	-0.01497	-0.01586	1.85739
A48	1.85829	-0.00023	0.00059	-0.02622	-0.02602	1.83227
D1	-0.00076	-0.00002	-0.00004	-0.00184	-0.00189	-0.00265
D2	3.13537	-0.00001	-0.00019	-0.00049	-0.00067	3.13470
D3	-3.13898	0.00000	-0.00046	-0.00016	-0.00062	-3.13960
D4	-0.00285	0.00001	-0.00060	0.00118	0.00060	-0.00225
D5	0.00862	0.00001	0.00004	0.00024	0.00028	0.00891
D6	-3.13073	0.00001	0.00055	0.00008	0.00064	-3.13009
D7	-3.13632	-0.00002	0.00045	-0.00138	-0.00092	-3.13724
D8	0.00750	-0.00001	0.00096	-0.00154	-0.00056	0.00694
D9	-0.01182	0.00000	0.00011	0.00021	0.00032	-0.01150
D10	3.12705	-0.00002	0.00000	-0.00088	-0.00087	3.12618
D11	3.13512	-0.00001	0.00025	-0.00120	-0.00094	3.13418
D12	-0.00920	-0.00003	0.00015	-0.00229	-0.00213	-0.01132
D13	0.01623	0.00004	-0.00015	0.00265	0.00249	0.01872
D14	-3.13170	-0.00003	0.00024	-0.00213	-0.00188	-3.13358
D15	-3.12268	0.00006	-0.00005	0.00374	0.00368	-3.11900
D16	0.01257	-0.00001	0.00035	-0.00104	-0.00068	0.01188
D17	-3.12412	0.00004	0.00161	0.00051	0.00209	-3.12203
D18	0.00816	0.00001	0.00151	-0.00128	0.00021	0.00837
D19	0.01475	0.00002	0.00150	-0.00056	0.00093	0.01568
D20	-3.13615	-0.00001	0.00140	-0.00235	-0.00095	-3.13711

D21	-0.00881	-0.00005	0.00015	-0.00423	-0.00405	-0.01286
D22	3.11789	-0.00004	0.00049	-0.00325	-0.00274	3.11515
D23	3.13932	0.00002	-0.00027	0.00076	0.00052	3.13984
D24	-0.01716	0.00003	0.00007	0.00174	0.00183	-0.01533
D25	-0.04002	-0.00001	-0.00265	0.00267	0.00002	-0.04001
D26	3.11453	0.00004	-0.00336	0.00632	0.00299	3.11752
D27	3.09485	-0.00008	-0.00222	-0.00251	-0.00478	3.09007
D28	-0.03378	-0.00003	-0.00293	0.00113	-0.00181	-0.03559
D29	-0.00357	0.00003	-0.00010	0.00290	0.00280	-0.00077
D30	3.13578	0.00003	-0.00062	0.00305	0.00244	3.13822
D31	-3.13039	0.00002	-0.00042	0.00175	0.00136	-3.12903
D32	0.00896	0.00002	-0.00093	0.00191	0.00099	0.00995
D33	-0.01410	-0.00002	-0.00102	0.00048	-0.00054	-0.01465
D34	3.12383	-0.00002	-0.00172	0.00064	-0.00107	3.12276
D35	3.13680	0.00001	-0.00092	0.00226	0.00132	3.13812
D36	-0.00845	0.00001	-0.00162	0.00242	0.00080	-0.00765
D37	0.04061	0.00001	0.00310	-0.00254	0.00055	0.04117
D38	-3.09153	0.00001	0.00441	-0.00356	0.00085	-3.09068
D39	-3.11406	-0.00003	0.00373	-0.00591	-0.00216	-3.11623
D40	0.03698	-0.00004	0.00504	-0.00693	-0.00187	0.03511
D41	1.47169	-0.00005	-0.04148	-0.00185	-0.04333	1.42836
D42	-2.70532	-0.00010	-0.03809	-0.01004	-0.04829	-2.75360
D43	-0.62489	-0.00006	-0.03832	-0.00453	-0.04272	-0.66762
D44	-1.65680	0.00000	-0.04216	0.00173	-0.04041	-1.69722
D45	0.44937	-0.00005	-0.03877	-0.00647	-0.04537	0.40400
D46	2.52979	-0.00001	-0.03899	-0.00095	-0.03981	2.48999

```
   D47       -0.01385   0.00000  -0.00131   0.00096  -0.00034  -
0.01420
   D48        3.13134   0.00001  -0.00062   0.00083   0.00021
3.13155
   D49        3.11886   0.00000  -0.00253   0.00192  -0.00061
3.11824
   D50       -0.01913   0.00001  -0.00184   0.00178  -0.00006  -
0.01920
   D51       -3.13949   0.00001   0.00031   0.00119   0.00149  -
3.13800
   D52        0.01846  -0.00002   0.00098  -0.00178  -0.00081
0.01765
   D53        0.01131   0.00001   0.00159   0.00011   0.00170
0.01300
   D54       -3.11393  -0.00002   0.00226  -0.00285  -0.00060  -
3.11453
   D55        0.01115   0.00000   0.00108  -0.00010   0.00096
0.01211
   D56       -3.12465  -0.00001   0.00158  -0.00229  -0.00072  -
3.12537
   D57       -3.13410   0.00000   0.00038   0.00004   0.00041  -
3.13369
   D58        0.01329  -0.00002   0.00088  -0.00215  -0.00127
0.01202
   D59        0.00131   0.00001   0.00045   0.00060   0.00104
0.00236
   D60        3.13840   0.00001   0.00021   0.00092   0.00113
3.13953
   D61       -3.13436  -0.00001   0.00095  -0.00154  -0.00061  -
3.13496
   D62        0.00273  -0.00001   0.00071  -0.00121  -0.00052
0.00222
   D63       -0.00966   0.00001  -0.00075   0.00143   0.00067  -
0.00899
   D64        3.12917   0.00001  -0.00171   0.00217   0.00046
3.12963
   D65        3.13642   0.00001  -0.00051   0.00103   0.00052
3.13693
   D66       -0.00794   0.00001  -0.00147   0.00178   0.00031  -
0.00763
   D67        0.00300  -0.00002  -0.00031  -0.00175  -0.00206
0.00095
   D68        3.12842   0.00001  -0.00096   0.00123   0.00027
3.12869
   D69       -3.13582  -0.00002   0.00065  -0.00249  -0.00184  -
3.13766
   D70       -0.01040   0.00001   0.00000   0.00049   0.00048  -
0.00992
         Item               Value     Threshold  Converged?
 Maximum Force            0.000353     0.000450     YES
 RMS     Force            0.000100     0.000300     YES
 Maximum Displacement     0.119117     0.001800     NO
```

This journal is © The Royal Society of Chemistry 2014

```
 RMS     Displacement     0.020656     0.001200     NO
 Predicted change in Energy=-1.554347D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.786733   -5.443417    0.012769
      2          6           0       -3.421676   -5.396812   -0.015406
      3          6           0       -2.718564   -4.149484   -0.030091
      4          6           0       -3.449424   -2.907290   -0.029524
      5          6           0       -4.882366   -3.010265    0.010391
      6          6           0       -5.523110   -4.221191    0.031095
      7          6           0       -1.318692   -4.122852   -0.040383
      8          6           0       -2.752542   -1.671234   -0.053915
      9          6           0       -1.345114   -1.670947   -0.029515
     10          6           0       -0.616066   -2.914268   -0.031387
     11          6           0        0.816651   -2.902346   -0.018888
     12          1           0        1.326121   -3.867528   -0.028497
     13          6           0        1.517833   -1.729662    0.008945
     14          6           0        0.802705   -0.492503    0.028782
     15          6           0       -0.566132   -0.468189    0.009752
     16          1           0       -0.764444   -5.063211   -0.045086
     17          1           0       -5.321110   -6.391876    0.025786
     18          1           0       -2.824793   -6.310562   -0.023632
     19          1           0       -5.490325   -2.111026    0.037793
     20          1           0       -6.612794   -4.256415    0.064539
     21          1           0        2.606392   -1.720346    0.020360
     22          1           0        1.358415    0.445435    0.062390
     23          1           0       -1.065348    0.499364    0.038510
     24          6           0       -3.499547   -0.371392   -0.084675
     25          1           0       -3.832050   -0.067593    0.917563
     26          1           0       -2.913136    0.460812   -0.479276
     27          1           0       -4.395582   -0.407216   -0.709882
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1          2          3          4          5
    1  C    0.000000
    2  C    1.366143   0.000000
    3  C    2.439963   1.431925   0.000000
    4  C    2.867425   2.489717   1.441251   0.000000
    5  C    2.435032   2.798194   2.445710   1.437192   0.000000
    6  C    1.427033   2.408376   2.806129   2.455644   1.370154
    7  C    3.711337   2.458890   1.400163   2.453106   3.733657
    8  C    4.286228   3.785387   2.478598   1.419181   2.516603
    9  C    5.106668   4.265487   2.833640   2.440628   3.782528
   10  C    4.877808   3.746295   2.438496   2.833367   4.267584
   11  C    6.152719   4.917905   3.748764   4.266091   5.700114
```

This journal is © The Royal Society of Chemistry 2014

12	H	6.312853	4.988032	4.054502	4.871128	6.267514
13	C	7.317072	6.152019	4.878947	5.105089	6.527059
14	C	7.466835	6.472990	5.077038	4.890316	6.217676
15	C	6.524292	5.696148	4.264563	3.776788	5.009195
16	H	4.040632	2.678255	2.157246	3.443451	4.601624
17	H	1.088715	2.144690	3.435794	3.955832	3.409988
18	H	2.145337	1.091455	2.163696	3.460124	3.889309
19	H	3.405951	3.883109	3.441305	2.191768	1.085817
20	H	2.178567	3.389709	3.896846	3.440334	2.133120
21	H	8.277657	7.060828	5.853070	6.171243	7.599045
22	H	8.511397	7.548985	6.143582	5.862126	7.133857
23	H	7.011849	6.349810	4.934534	4.158574	5.185356
24	C	5.233716	5.026501	3.858354	2.536992	2.980751
25	H	5.534398	5.425811	4.335866	3.017823	3.253529
26	H	6.213887	5.897928	4.636212	3.440057	4.020699
27	H	5.102798	5.130971	4.156811	2.758345	2.744379

		6	7	8	9	10
6	C	0.000000				
7	C	4.206175	0.000000			
8	C	3.766372	2.840165	0.000000		
9	C	4.895209	2.452071	1.407639	0.000000	
10	C	5.078487	1.398013	2.471876	1.441306	0.000000
11	C	6.475679	2.459632	3.775712	2.487909	1.432821
12	H	6.858615	2.657136	4.632477	3.458391	2.163517
13	C	7.468808	3.711558	4.271237	2.863808	2.440992
14	C	7.342959	4.205299	3.746468	2.450562	2.807397
15	C	6.217485	3.731678	2.496349	1.433521	2.446935
16	H	4.833188	1.091554	3.931681	3.441639	2.154103
17	H	2.180069	4.601325	5.374788	6.172420	5.851022
18	H	3.413119	2.656068	4.639989	4.869858	4.051339
19	H	2.110431	4.632071	2.774398	4.169049	4.940485
20	H	1.090765	5.296825	4.647444	5.868725	6.145836
21	H	8.505478	4.602392	5.359674	3.952130	3.436912
22	H	8.314672	5.295914	4.625341	3.434616	3.898073
23	H	6.492715	4.629826	2.750757	2.189326	3.443781
24	C	4.350766	4.339532	1.499517	2.516637	3.844934
25	H	4.571421	4.866184	2.163509	3.106855	4.398479
26	H	5.384570	4.872869	2.179987	2.684283	4.107104
27	H	4.045587	4.870465	2.174308	3.371241	4.585892

		11	12	13	14	15
11	C	0.000000				
12	H	1.091434	0.000000			
13	C	1.366609	2.146771	0.000000		
14	C	2.410355	3.415851	1.429113	0.000000	
15	C	2.799649	3.890706	2.436026	1.369185	0.000000
16	H	2.677664	2.408401	4.040329	4.832472	4.599627
17	H	7.060519	7.110623	8.276935	8.503159	7.596061
18	H	4.987592	4.816485	6.312219	6.856479	6.263864
19	H	6.356678	7.039435	7.018586	6.497840	5.191087
20	H	7.552292	7.948978	8.514380	8.316125	7.135530
21	H	2.145189	2.500374	1.088659	2.181962	3.410707
22	H	3.392308	4.314042	2.181586	1.090720	2.131046

23	H	3.888040	4.979294	3.412075	2.115069	1.089129
24	C	5.003961	5.959295	5.198823	4.305451	2.936530
25	H	5.524779	6.476208	5.675324	4.738294	3.413329
26	H	5.043224	6.075281	4.966893	3.869678	2.571113
27	H	5.819839	6.721305	6.101971	5.251198	3.896958

		16	17	18	19	20
16	H	0.000000				
17	H	4.746954	0.000000			
18	H	2.408606	2.498130	0.000000		
19	H	5.572811	4.284210	4.974429	0.000000	
20	H	5.904755	2.496024	4.310016	2.421435	0.000000
21	H	4.747796	9.201549	7.111244	8.106156	9.561746
22	H	5.904512	9.558567	7.946705	7.310358	9.254597
23	H	5.571335	8.099436	7.033819	5.137563	7.307001
24	C	5.430978	6.290987	5.977688	2.646606	4.980760
25	H	5.940800	6.558134	6.393362	2.774796	5.099649
26	H	5.943083	7.280986	6.787262	3.677446	6.019588
27	H	5.941835	6.100324	6.147179	2.158807	4.509112

		21	22	23	24	25
21	H	0.000000				
22	H	2.499964	0.000000			
23	H	4.290585	2.424481	0.000000		
24	C	6.254055	4.928349	2.588188	0.000000	
25	H	6.707466	5.285399	2.957839	1.098787	0.000000
26	H	5.955861	4.305785	1.919351	1.091857	1.753503
27	H	7.161369	5.867870	3.531634	1.093182	1.755417

		26	27
26	H	0.000000	
27	H	1.733291	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.662655	-0.996160	0.020927
2	6	0	-2.463924	-1.650708	-0.010006
3	6	0	-1.223814	-0.934870	-0.020528
4	6	0	-1.220640	0.506357	-0.012703
5	6	0	-2.506502	1.146877	0.029861
6	6	0	-3.674402	0.430597	0.046432
7	6	0	-0.005289	-1.624420	-0.033745
8	6	0	0.008375	1.215712	-0.032969
9	6	0	1.219978	0.499465	-0.011630
10	6	0	1.214671	-0.941803	-0.020763
11	6	0	2.453970	-1.660848	-0.011327
12	1	0	2.401234	-2.750902	-0.026449

```
     13          6           0        3.654406   -1.008491    0.020331
     14          6           0        3.668550    0.420296    0.047370
     15          6           0        2.502685    1.138050    0.031430
     16          1           0       -0.006850   -2.715925   -0.043945
     17          1           0       -4.605399   -1.540621    0.030778
     18          1           0       -2.415240   -2.740992   -0.023701
     19          1           0       -2.572114    2.230212    0.062689
     20          1           0       -4.630310    0.954751    0.082087
     21          1           0        4.596139   -1.554600    0.029419
     22          1           0        4.624281    0.944609    0.084048
     23          1           0        2.565446    2.224830    0.065689
     24          6           0        0.027009    2.714934   -0.056171
     25          1           0       -0.105016    3.140626    0.948164
     26          1           0        0.955540    3.134766   -0.448246
     27          1           0       -0.762223    3.143323   -0.679583
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3984611      0.4488490
0.3405999
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       880.0014098102 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.859669647     A.U. after   12 cycles
             Convg  =    0.9428D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.004527492    0.001577480    0.000088277
      2        6           0.005084114   -0.002305968   -0.000184085
      3        6           0.004866852   -0.002273938    0.000029988
      4        6          -0.004478602    0.000394571    0.000248754
      5        6           0.000149491    0.005232043   -0.000291705
      6        6          -0.003246360   -0.003946552    0.000109272
      7        6           0.000480159   -0.000897822    0.000005806
      8        6          -0.002480070   -0.005214520   -0.001334925
      9        6           0.005645693    0.002230833    0.000066240
     10        6           0.001256489   -0.005166879    0.000096121
     11        6          -0.000227570   -0.005099155   -0.000162665
     12        1           0.000129109    0.002626615    0.000061680
     13        6          -0.000089570    0.004586570    0.000068552
```

```
     14        6           0.005472550    0.000833323    0.000175084
     15        6          -0.001349375    0.005845350    0.000069907
     16        1          -0.001177470    0.001696476   -0.000028418
     17        1           0.001556234    0.000687050   -0.000021752
     18        1          -0.002166753    0.001315821    0.000047719
     19        1           0.001567856    0.000782587   -0.000288507
     20        1           0.002360388    0.000434320   -0.000033239
     21        1          -0.001349764   -0.001010301   -0.000020949
     22        1          -0.001160764   -0.002016384   -0.000053317
     23        1           0.002113395   -0.003444144   -0.000002281
     24        6          -0.008327161    0.008796133    0.000744015
     25        1          -0.000339470   -0.000372291    0.001287992
     26        1           0.001547962   -0.001953612   -0.000125085
     27        1          -0.001309872   -0.003337606   -0.000552479
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.008796133 RMS     0.002709406


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.010432484 RMS     0.002037087
 Search for a local minimum.
 Step number  21 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
21
                                                     20
 DE=  9.01D-04 DEPred=-1.55D-03 R=-5.80D-01
 Trust test=-5.80D-01 RLast= 1.42D-01 DXMaxT set to 5.03D-02
 Use linear search instead of GDIIS.
 Quartic linear search produced a step of -0.94346.
 Iteration  1 RMS(Cart)=  0.01942378 RMS(Int)=  0.00035069
 Iteration  2 RMS(Cart)=  0.00039711 RMS(Int)=  0.00000263
 Iteration  3 RMS(Cart)=  0.00000014 RMS(Int)=  0.00000262
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58164   0.00378   0.00832   0.00000   0.00832
2.58995
    R2        2.69670  -0.00041  -0.00516   0.00000  -0.00516
2.69154
    R3        2.05737  -0.00136  -0.00333   0.00000  -0.00333
2.05404
```

This journal is © The Royal Society of Chemistry 2014

R4	2.70595	0.00020	-0.00142	0.00000	-0.00143
2.70452					
R5	2.06255	-0.00229	-0.00653	0.00000	-0.00653
2.05602					
R6	2.72357	0.00261	0.01101	0.00000	0.01101
2.73458					
R7	2.64593	-0.00066	-0.00384	0.00000	-0.00384
2.64208					
R8	2.71590	-0.00194	-0.00400	0.00000	-0.00400
2.71190					
R9	2.68186	-0.00267	-0.00239	0.00000	-0.00239
2.67948					
R10	2.58922	0.00224	0.00586	0.00000	0.00586
2.59508					
R11	2.05190	-0.00024	-0.00293	0.00000	-0.00293
2.04897					
R12	2.06125	-0.00237	-0.00671	0.00000	-0.00671
2.05454					
R13	2.64186	0.00008	-0.00021	0.00000	-0.00021
2.64166					
R14	2.06274	-0.00206	-0.00560	0.00000	-0.00560
2.05714					
R15	2.66005	0.01043	0.01895	0.00000	0.01895
2.67900					
R16	2.83368	0.00689	0.02805	0.00000	0.02805
2.86173					
R17	2.72367	0.00543	0.01333	0.00000	0.01333
2.73700					
R18	2.70896	0.00396	0.00380	0.00000	0.00380
2.71276					
R19	2.70764	0.00018	-0.00265	0.00000	-0.00265
2.70499					
R20	2.06251	-0.00226	-0.00651	0.00000	-0.00651
2.05600					
R21	2.58252	0.00208	0.00686	0.00000	0.00686
2.58937					
R22	2.70063	-0.00200	-0.00893	0.00000	-0.00893
2.69170					
R23	2.05727	-0.00136	-0.00324	0.00000	-0.00324
2.05402					
R24	2.58738	0.00260	0.00716	0.00000	0.00716
2.59454					
R25	2.06116	-0.00233	-0.00663	0.00000	-0.00663
2.05453					
R26	2.05816	-0.00403	-0.00955	0.00000	-0.00955
2.04860					
R27	2.07641	0.00118	0.00131	0.00000	0.00131
2.07771					
R28	2.06331	-0.00061	-0.00021	0.00000	-0.00021
2.06310					
R29	2.06581	0.00150	0.00037	0.00000	0.00037
2.06619					

This journal is © The Royal Society of Chemistry 2014

A1	2.07905	0.00181	0.01053	0.00000	0.01053
2.08958					
A2	2.11813	-0.00195	-0.01661	0.00000	-0.01661
2.10151					
A3	2.08600	0.00014	0.00609	0.00000	0.00609
2.09208					
A4	2.11831	-0.00066	-0.00201	0.00000	-0.00201
2.11629					
A5	2.11534	-0.00080	-0.01187	0.00000	-0.01187
2.10347					
A6	2.04953	0.00146	0.01388	0.00000	0.01388
2.06341					
A7	2.09644	-0.00270	-0.01161	0.00000	-0.01161
2.08484					
A8	2.10316	0.00196	0.00992	0.00000	0.00992
2.11307					
A9	2.08358	0.00074	0.00169	0.00000	0.00169
2.08527					
A10	2.03070	0.00385	0.01361	0.00000	0.01361
2.04431					
A11	2.09631	0.00111	-0.00184	0.00000	-0.00184
2.09447					
A12	2.15613	-0.00496	-0.01174	0.00000	-0.01174
2.14439					
A13	2.12940	-0.00142	-0.00516	0.00000	-0.00516
2.12424					
A14	2.09395	-0.00108	-0.00670	0.00000	-0.00670
2.08725					
A15	2.05975	0.00250	0.01185	0.00000	0.01184
2.07160					
A16	2.11232	-0.00088	-0.00532	0.00000	-0.00532
2.10699					
A17	2.08087	0.00081	0.00588	0.00000	0.00588
2.08675					
A18	2.08999	0.00007	-0.00056	0.00000	-0.00056
2.08944					
A19	2.11634	0.00067	0.00283	0.00000	0.00283
2.11917					
A20	2.08438	-0.00049	-0.00224	0.00000	-0.00224
2.08214					
A21	2.08241	-0.00018	-0.00058	0.00000	-0.00058
2.08184					
A22	2.08386	-0.00013	0.00391	0.00000	0.00390
2.08777					
A23	2.10682	-0.00878	-0.01629	0.00000	-0.01629
2.09053					
A24	2.09240	0.00891	0.01242	0.00000	0.01242
2.10481					
A25	2.10082	-0.00324	-0.00915	0.00000	-0.00915
2.09167					
A26	2.14596	0.00391	0.00343	0.00000	0.00343
2.14939					

A27	2.03637	-0.00067	0.00572	0.00000	0.00572	2.04209
A28	2.08465	0.00084	0.00258	0.00000	0.00258	2.08723
A29	2.10575	-0.00008	0.00478	0.00000	0.00478	2.11053
A30	2.09278	-0.00077	-0.00735	0.00000	-0.00735	2.08542
A31	2.04803	0.00135	0.01482	0.00000	0.01482	2.06285
A32	2.11807	0.00007	-0.00121	0.00000	-0.00122	2.11686
A33	2.11708	-0.00142	-0.01361	0.00000	-0.01361	2.10347
A34	2.07874	0.00189	0.01009	0.00000	0.01009	2.08883
A35	2.11834	-0.00197	-0.01641	0.00000	-0.01641	2.10193
A36	2.08610	0.00008	0.00631	0.00000	0.00631	2.09241
A37	2.11233	-0.00030	-0.00478	0.00000	-0.00477	2.10756
A38	2.08277	0.00012	0.00398	0.00000	0.00398	2.08675
A39	2.08808	0.00018	0.00080	0.00000	0.00080	2.08887
A40	2.12792	-0.00022	-0.00247	0.00000	-0.00247	2.12545
A41	2.09095	0.00042	-0.00203	0.00000	-0.00204	2.08891
A42	2.06423	-0.00020	0.00448	0.00000	0.00447	2.06871
A43	1.95164	0.00032	-0.00071	0.00000	-0.00071	1.95094
A44	1.98292	-0.00225	-0.02619	0.00000	-0.02618	1.95674
A45	1.97322	-0.00374	-0.02599	0.00000	-0.02598	1.94724
A46	1.85609	0.00167	0.01838	0.00000	0.01838	1.87446
A47	1.85739	0.00136	0.01496	0.00000	0.01496	1.87235
A48	1.83227	0.00326	0.02455	0.00000	0.02457	1.85684
D1	-0.00265	0.00008	0.00178	0.00000	0.00178	-0.00087
D2	3.13470	0.00009	0.00063	0.00000	0.00063	3.13533
D3	-3.13960	0.00001	0.00058	0.00000	0.00058	-3.13902
D4	-0.00225	0.00002	-0.00057	0.00000	-0.00057	-0.00282

This journal is © The Royal Society of Chemistry 2014

D5	0.00891	-0.00003	-0.00027	0.00000	-0.00027	0.00864
D6	-3.13009	-0.00007	-0.00060	0.00000	-0.00060	-3.13070
D7	-3.13724	0.00002	0.00087	0.00000	0.00087	-3.13638
D8	0.00694	-0.00001	0.00053	0.00000	0.00053	0.00747
D9	-0.01150	0.00003	-0.00030	0.00000	-0.00030	-0.01180
D10	3.12618	0.00010	0.00082	0.00000	0.00082	3.12700
D11	3.13418	0.00003	0.00088	0.00000	0.00088	3.13506
D12	-0.01132	0.00010	0.00201	0.00000	0.00201	-0.00932
D13	0.01872	-0.00011	-0.00234	0.00000	-0.00234	0.01638
D14	-3.13358	0.00003	0.00177	0.00000	0.00177	-3.13181
D15	-3.11900	-0.00018	-0.00347	0.00000	-0.00347	-3.12247
D16	0.01188	-0.00004	0.00065	0.00000	0.00064	0.01253
D17	-3.12203	-0.00004	-0.00197	0.00000	-0.00197	-3.12400
D18	0.00837	0.00001	-0.00020	0.00000	-0.00020	0.00818
D19	0.01568	0.00002	-0.00088	0.00000	-0.00087	0.01480
D20	-3.13711	0.00007	0.00090	0.00000	0.00090	-3.13621
D21	-0.01286	0.00014	0.00382	0.00000	0.00382	-0.00904
D22	3.11515	0.00020	0.00259	0.00000	0.00259	3.11774
D23	3.13984	-0.00005	-0.00049	0.00000	-0.00049	3.13935
D24	-0.01533	0.00001	-0.00173	0.00000	-0.00173	-0.01706
D25	-0.04001	0.00008	-0.00001	0.00000	-0.00001	-0.04002
D26	3.11752	0.00001	-0.00282	0.00000	-0.00282	3.11470
D27	3.09007	0.00029	0.00451	0.00000	0.00451	3.09458
D28	-0.03559	0.00022	0.00170	0.00000	0.00171	-0.03388
D29	-0.00077	-0.00009	-0.00265	0.00000	-0.00265	-0.00341
D30	3.13822	-0.00006	-0.00230	0.00000	-0.00230	3.13592

This journal is © The Royal Society of Chemistry 2014

D31	-3.12903	-0.00012	-0.00128	0.00000	-0.00128	-3.13032
D32	0.00995	-0.00009	-0.00093	0.00000	-0.00094	0.00902
D33	-0.01465	0.00006	0.00051	0.00000	0.00051	-0.01413
D34	3.12276	0.00004	0.00101	0.00000	0.00101	3.12377
D35	3.13812	0.00002	-0.00125	0.00000	-0.00125	3.13688
D36	-0.00765	-0.00001	-0.00075	0.00000	-0.00075	-0.00840
D37	0.04117	-0.00009	-0.00052	0.00000	-0.00052	0.04064
D38	-3.09068	0.00004	-0.00080	0.00000	-0.00080	-3.09148
D39	-3.11623	-0.00019	0.00204	0.00000	0.00204	-3.11419
D40	0.03511	-0.00006	0.00176	0.00000	0.00176	0.03687
D41	1.42836	-0.00019	0.04088	0.00000	0.04088	1.46924
D42	-2.75360	0.00061	0.04556	0.00000	0.04556	-2.70804
D43	-0.66762	0.00046	0.04031	0.00000	0.04030	-0.62732
D44	-1.69722	-0.00017	0.03813	0.00000	0.03813	-1.65909
D45	0.40400	0.00063	0.04281	0.00000	0.04281	0.44681
D46	2.48999	0.00048	0.03756	0.00000	0.03755	2.52754
D47	-0.01420	0.00001	0.00032	0.00000	0.00032	-0.01387
D48	3.13155	0.00004	-0.00020	0.00000	-0.00020	3.13135
D49	3.11824	-0.00009	0.00058	0.00000	0.00058	3.11882
D50	-0.01920	-0.00006	0.00006	0.00000	0.00006	-0.01914
D51	-3.13800	-0.00011	-0.00141	0.00000	-0.00141	-3.13941
D52	0.01765	-0.00003	0.00076	0.00000	0.00076	0.01841
D53	0.01300	0.00004	-0.00160	0.00000	-0.00160	0.01140
D54	-3.11453	0.00011	0.00057	0.00000	0.00057	-3.11397
D55	0.01211	0.00003	-0.00091	0.00000	-0.00091	0.01120
D56	-3.12537	0.00007	0.00068	0.00000	0.00068	-3.12469

```
   D57       -3.13369   0.00000  -0.00039   0.00000  -0.00039  -
3.13407
   D58        0.01202   0.00005   0.00120   0.00000   0.00120
0.01322
   D59        0.00236   0.00001  -0.00098   0.00000  -0.00098
0.00137
   D60        3.13953  -0.00003  -0.00107   0.00000  -0.00107
3.13847
   D61       -3.13496   0.00005   0.00057   0.00000   0.00057  -
3.13439
   D62        0.00222   0.00001   0.00049   0.00000   0.00049
0.00271
   D63       -0.00899  -0.00005  -0.00063   0.00000  -0.00063  -
0.00962
   D64        3.12963  -0.00006  -0.00043   0.00000  -0.00043
3.12919
   D65        3.13693   0.00000  -0.00049   0.00000  -0.00049
3.13645
   D66       -0.00763  -0.00001  -0.00029   0.00000  -0.00029  -
0.00793
   D67        0.00095   0.00001   0.00194   0.00000   0.00194
0.00289
   D68        3.12869  -0.00006  -0.00025   0.00000  -0.00025
3.12844
   D69       -3.13766   0.00002   0.00174   0.00000   0.00174  -
3.13592
   D70       -0.00992  -0.00005  -0.00046   0.00000  -0.00046  -
0.01038
         Item               Value     Threshold  Converged?
 Maximum Force            0.010432     0.000450     NO
 RMS     Force            0.002037     0.000300     NO
 Maximum Displacement     0.112325     0.001800     NO
 RMS     Displacement     0.019485     0.001200     NO
 Predicted change in Energy=-3.536322D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792511   -5.429087    0.009796
      2          6           0       -3.422627   -5.396697   -0.017741
      3          6           0       -2.709282   -4.156030   -0.029234
      4          6           0       -3.446946   -2.911090   -0.026343
      5          6           0       -4.878891   -2.998971    0.009094
      6          6           0       -5.527522   -4.209232    0.028520
      7          6           0       -1.311484   -4.127467   -0.039864
      8          6           0       -2.752250   -1.675232   -0.049646
      9          6           0       -1.334795   -1.667665   -0.026384
```

10	6	0	-0.607186	-2.919988	-0.030137
11	6	0	0.824096	-2.903285	-0.019297
12	1	0	1.349344	-3.856034	-0.029575
13	6	0	1.521781	-1.724335	0.010067
14	6	0	0.815860	-0.487375	0.032032
15	6	0	-0.556741	-0.461907	0.012777
16	1	0	-0.759537	-5.065727	-0.047126
17	1	0	-5.320255	-6.379262	0.020639
18	1	0	-2.848158	-6.320630	-0.026412
19	1	0	-5.470576	-2.090744	0.034988
20	1	0	-6.613882	-4.238003	0.060652
21	1	0	2.608663	-1.727925	0.020893
22	1	0	1.371240	0.446623	0.067039
23	1	0	-1.057217	0.499250	0.043078
24	6	0	-3.529574	-0.375992	-0.081845
25	1	0	-3.832998	-0.057048	0.925658
26	1	0	-2.950655	0.438493	-0.521595
27	1	0	-4.439327	-0.466656	-0.681517

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370543	0.000000			
3	C	2.441729	1.431170	0.000000		
4	C	2.855199	2.485742	1.447077	0.000000	
5	C	2.431651	2.805444	2.459158	1.435077	0.000000
6	C	1.424303	2.417188	2.819334	2.452954	1.373256
7	C	3.716750	2.463404	1.398131	2.457632	3.741964
8	C	4.272894	3.781498	2.481254	1.417918	2.505661
9	C	5.109344	4.273733	2.842742	2.450976	3.786060
10	C	4.879971	3.749794	2.438567	2.839777	4.272615
11	C	6.158473	4.924608	3.748897	4.271055	5.703860
12	H	6.340223	5.014528	4.069698	4.888489	6.287047
13	C	7.320893	6.159074	4.880224	5.108616	6.526354
14	C	7.474947	6.486038	5.088163	4.904010	6.224052
15	C	6.527988	5.706697	4.275715	3.788576	5.011755
16	H	4.049710	2.683739	2.151599	3.444570	4.609091
17	H	1.086952	2.137264	3.429640	3.942045	3.409004
18	H	2.139315	1.087999	2.169053	3.461721	3.893399
19	H	3.406603	3.889242	3.448808	2.184447	1.084268
20	H	2.176847	3.396002	3.906495	3.434786	2.132617
21	H	8.275029	7.059593	5.846260	6.170293	7.594680
22	H	8.515813	7.558621	6.151776	5.873489	7.137199
23	H	7.007047	6.353035	4.940261	4.164858	5.181109
24	C	5.209335	5.022253	3.868376	2.537051	2.951092
25	H	5.533378	5.437855	4.356169	3.033298	3.254058
26	H	6.172788	5.875889	4.627129	3.422175	3.976919
27	H	5.022785	5.077360	4.126743	2.718332	2.661349

		6	7	8	9	10
6	C	0.000000				
7	C	4.217386	0.000000			
8	C	3.758910	2.844180	0.000000		

This journal is © The Royal Society of Chemistry 2014

9	C	4.903217	2.459949	1.417666	0.000000	
10	C	5.086777	1.397904	2.480141	1.448358	0.000000
11	C	6.484662	2.461655	3.781440	2.487492	1.431420
12	H	6.886176	2.674656	4.645361	3.463173	2.168915
13	C	7.474472	3.715498	4.274730	2.857371	2.442069
14	C	7.354640	4.216756	3.761527	2.453938	2.818959
15	C	6.225059	3.742825	2.509246	1.435533	2.458973
16	H	4.844894	1.088591	3.932731	3.446473	2.151208
17	H	2.179920	4.598314	5.359803	6.171325	5.846553
18	H	3.411746	2.677968	4.646447	4.892888	4.072633
19	H	2.119263	4.631619	2.751201	4.157818	4.934010
20	H	1.087216	5.304503	4.635964	5.872220	6.150269
21	H	8.506143	4.596634	5.361637	3.944202	3.430059
22	H	8.322944	5.303842	4.638864	3.435342	3.906108
23	H	6.492584	4.634441	2.758642	2.185726	3.449504
24	C	4.324084	4.358354	1.514362	2.547263	3.874912
25	H	4.573500	4.884525	2.176638	3.121136	4.417673
26	H	5.342679	4.875135	2.174841	2.700397	4.124655
27	H	3.961716	4.857640	2.169366	3.392602	4.596569

		11	12	13	14	15
11	C	0.000000				
12	H	1.087989	0.000000			
13	C	1.370237	2.139029	0.000000		
14	C	2.416469	3.411196	1.424386	0.000000	
15	C	2.805008	3.892949	2.431869	1.372972	0.000000
16	H	2.680452	2.431264	4.046305	4.842463	4.608674
17	H	7.059537	7.131112	8.275380	8.506842	7.596461
18	H	5.016348	4.867573	6.342210	6.888781	6.291007
19	H	6.347131	7.044979	7.001995	6.487687	5.176812
20	H	7.557208	7.972892	8.515287	8.322806	7.137938
21	H	2.137233	2.473314	1.086942	2.180190	3.409201
22	H	3.395395	4.303797	2.176917	1.087210	2.132014
23	H	3.888505	4.976476	3.405385	2.117066	1.084074
24	C	5.034438	5.993101	5.229021	4.348352	2.975579
25	H	5.539182	6.496263	5.682588	4.753486	3.425072
26	H	5.066412	6.097134	4.996316	3.917955	2.612872
27	H	5.837750	6.739557	6.131465	5.303450	3.944179

		16	17	18	19	20
16	H	0.000000				
17	H	4.746590	0.000000			
18	H	2.436709	2.473240	0.000000		
19	H	5.572357	4.291176	4.977227	0.000000	
20	H	5.913553	2.502012	4.304137	2.432803	0.000000
21	H	4.742396	9.192534	7.132467	8.087394	9.558108
22	H	5.910943	9.558817	7.975448	7.297240	9.257858
23	H	5.573663	8.092461	7.051458	5.117214	7.301945
24	C	5.446827	6.265484	5.983822	2.592588	4.944531
25	H	5.956454	6.557544	6.411615	2.758782	5.095286
26	H	5.943279	7.238150	6.778013	3.613423	5.968908
27	H	5.924084	6.018967	6.101639	2.052928	4.416171

		21	22	23	24	25
21	H	0.000000				

```
   22  H    2.502400   0.000000
   23  H    4.289461   2.429145   0.000000
   24  C    6.286194   4.971603   2.625682   0.000000
   25  H    6.716057   5.298585   2.965363   1.099479   0.000000
   26  H    5.991134   4.361804   1.976779   1.091748   1.765965
   27  H    7.194328   5.929343   3.591196   1.093380   1.765907
                 26         27
   26  H    0.000000
   27  H    1.749576   0.000000
 Stoichiometry    C15H12
 Framework group  C1[X(C15H12)]
 Deg. of freedom    75
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.658338   -0.996439    0.020715
      2          6           0       -2.459924   -1.660707   -0.009917
      3          6           0       -1.217359   -0.950635   -0.018758
      4          6           0       -1.224684    0.496396   -0.009802
      5          6           0       -2.504694    1.144114    0.028683
      6          6           0       -3.676050    0.427539    0.045411
      7          6           0        0.003214   -1.632384   -0.032564
      8          6           0       -0.000645    1.211793   -0.030426
      9          6           0        1.226286    0.501850   -0.010458
     10          6           0        1.221205   -0.946466   -0.020279
     11          6           0        2.464681   -1.655461   -0.012734
     12          1           0        2.436388   -2.742981   -0.027562
     13          6           0        3.662552   -0.990900    0.019104
     14          6           0        3.678588    0.433122    0.047032
     15          6           0        2.507058    1.148884    0.031081
     16          1           0        0.005282   -2.720909   -0.044387
     17          1           0       -4.593937   -1.549651    0.029484
     18          1           0       -2.431181   -2.748246   -0.023153
     19          1           0       -2.556226    2.226729    0.059127
     20          1           0       -4.627986    0.951619    0.079988
     21          1           0        4.598595   -1.543347    0.027371
     22          1           0        4.629869    0.958216    0.083992
     23          1           0        2.560981    2.231056    0.065903
     24          6           0       -0.014759    2.725868   -0.056277
     25          1           0       -0.115122    3.150205    0.953040
     26          1           0        0.896308    3.137930   -0.494541
     27          1           0       -0.845750    3.109934   -0.654129
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3934440      0.4479168
0.3397702
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
```

```
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9184789464 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
```

```
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860574340     A.U. after   12 cycles
             Convg  =    0.9280D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6           0.000107261   -0.000135643   -0.000033212
      2          6          -0.000079577   -0.000154193    0.000061887
      3          6          -0.000045247    0.000159043    0.000034311
      4          6           0.000047023   -0.000059978   -0.000161252
      5          6          -0.000082007    0.000032639    0.000128050
      6          6          -0.000071720    0.000141561    0.000001593
      7          6           0.000096108   -0.000089563   -0.000030310
      8          6           0.000041824   -0.000066506   -0.000084436
      9          6          -0.000019697   -0.000086175    0.000004398
     10          6          -0.000104379   -0.000003935    0.000018844
     11          6           0.000232791    0.000046217    0.000045653
     12          1          -0.000094882   -0.000013918   -0.000007662
     13          6           0.000047935   -0.000215135   -0.000020000
     14          6          -0.000109923    0.000126362   -0.000010413
     15          6           0.000189949    0.000193469    0.000081026
     16          1          -0.000016150    0.000032204    0.000010626
     17          1          -0.000065301    0.000062031    0.000024752
     18          1           0.000051018    0.000073327   -0.000019068
     19          1           0.000019970    0.000032477    0.000010673
     20          1           0.000048703   -0.000053052   -0.000023148
     21          1          -0.000022757    0.000086198    0.000009488
     22          1           0.000019339   -0.000067490   -0.000017270
     23          1           0.000045299   -0.000062431   -0.000032572
     24          6          -0.000131940    0.000137933   -0.000032922
     25          1           0.000023307   -0.000051176   -0.000006528
     26          1          -0.000114137   -0.000060289    0.000097106
     27          1          -0.000012808   -0.000003976   -0.000049612
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000232791 RMS     0.000083563
```

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000346116 RMS     0.000067876
 Search for a local minimum.
 Step number  22 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
21
                                                     20   22
 Use linear search instead of GDIIS.
     Eigenvalues ---   -0.17009  -0.00256   0.00000   0.01272
0.01730
     Eigenvalues ---    0.01763   0.01811   0.01819   0.01866
0.01953
     Eigenvalues ---    0.01976   0.01991   0.01996   0.02047
0.02105
     Eigenvalues ---    0.02117   0.02139   0.02146   0.02214
0.02230
     Eigenvalues ---    0.02280   0.02357   0.02371   0.06163
0.06742
     Eigenvalues ---    0.08403   0.15448   0.15561   0.15923
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16003   0.16007
0.16039
     Eigenvalues ---    0.16192   0.18812   0.21278   0.21997
0.22584
     Eigenvalues ---    0.22800   0.23465   0.24330   0.24595
0.24986
     Eigenvalues ---    0.25279   0.26993   0.30160   0.30596
0.33570
     Eigenvalues ---    0.33593   0.33631   0.33682   0.33682
0.33709
     Eigenvalues ---    0.33809   0.34202   0.34460   0.36341
0.37040
     Eigenvalues ---    0.37242   0.38212   0.38770   0.39261
0.40317
     Eigenvalues ---    0.41039   0.41217   0.43777   0.44489
0.45083
     Eigenvalues ---    0.46347   0.48756   0.49695   0.49864
0.51317
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-1.70089931D-01 EMin=-1.70088981D-01
 RFO eigenvector is Hessian eigenvector with negative curvature.
 Taking step of  1.26D-01 in eigenvector direction.  Step.Grad= -
5.06D-05.
 Quartic linear search produced a step of -0.00029.
 Maximum step size (   0.050) exceeded in Quadratic search.
    -- Step size scaled by   0.400
 Iteration  1 RMS(Cart)=  0.00677543 RMS(Int)=  0.00004161
 Iteration  2 RMS(Cart)=  0.00004685 RMS(Int)=  0.00000972
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000972
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.58995   0.00001   0.00000  -0.00910  -0.00909
2.58086
    R2        2.69154   0.00010   0.00000   0.01347   0.01347
2.70501
    R3        2.05404  -0.00002   0.00000  -0.00107  -0.00107
2.05297
    R4        2.70452   0.00008   0.00000   0.00745   0.00745
2.71197
    R5        2.05602  -0.00003   0.00000  -0.00036  -0.00036
2.05566
    R6        2.73458  -0.00008   0.00000  -0.00650  -0.00651
2.72807
```

This journal is © The Royal Society of Chemistry 2014

R7	2.64208	0.00003	0.00000	0.00507	0.00507
2.64715					
R8	2.71190	0.00003	0.00000	0.00785	0.00785
2.71975					
R9	2.67948	-0.00004	0.00000	0.00161	0.00161
2.68109					
R10	2.59508	-0.00001	0.00000	-0.00535	-0.00535
2.58973					
R11	2.04897	0.00002	0.00000	0.00099	0.00099
2.04997					
R12	2.05454	-0.00005	0.00000	-0.00258	-0.00258
2.05196					
R13	2.64166	0.00001	0.00000	0.00363	0.00363
2.64528					
R14	2.05714	-0.00004	0.00000	-0.00107	-0.00107
2.05607					
R15	2.67900	0.00023	0.00000	-0.00364	-0.00364
2.67536					
R16	2.86173	0.00014	0.00000	-0.00094	-0.00094
2.86079					
R17	2.73700	0.00008	0.00000	-0.00352	-0.00352
2.73348					
R18	2.71276	0.00022	0.00000	0.00756	0.00755
2.72032					
R19	2.70499	0.00010	0.00000	0.00825	0.00826
2.71325					
R20	2.05600	-0.00003	0.00000	-0.00036	-0.00036
2.05564					
R21	2.58937	-0.00007	0.00000	-0.00961	-0.00961
2.57976					
R22	2.69170	0.00009	0.00000	0.01448	0.01448
2.70618					
R23	2.05402	-0.00002	0.00000	-0.00110	-0.00110
2.05292					
R24	2.59454	-0.00003	0.00000	-0.00623	-0.00623
2.58832					
R25	2.05453	-0.00005	0.00000	-0.00266	-0.00266
2.05187					
R26	2.04860	-0.00008	0.00000	0.00186	0.00186
2.05047					
R27	2.07771	-0.00003	0.00000	-0.00224	-0.00224
2.07548					
R28	2.06310	-0.00015	0.00000	-0.00269	-0.00269
2.06042					
R29	2.06619	0.00004	0.00000	0.00119	0.00119
2.06738					
A1	2.08958	-0.00001	0.00000	-0.00079	-0.00078
2.08880					
A2	2.10151	0.00009	0.00000	0.00550	0.00550
2.10702					
A3	2.09208	-0.00009	0.00000	-0.00472	-0.00472
2.08737					

This journal is © The Royal Society of Chemistry 2014

A4	2.11629	-0.00003	0.00000	-0.00379	-0.00379
2.11250					
A5	2.10347	0.00010	0.00000	0.00697	0.00697
2.11044					
A6	2.06341	-0.00007	0.00000	-0.00318	-0.00318
2.06022					
A7	2.08484	0.00002	0.00000	0.00557	0.00557
2.09040					
A8	2.11307	-0.00003	0.00000	-0.00503	-0.00502
2.10805					
A9	2.08527	0.00001	0.00000	-0.00055	-0.00055
2.08473					
A10	2.04431	0.00004	0.00000	-0.00027	-0.00027
2.04404					
A11	2.09447	0.00006	0.00000	0.00021	0.00022
2.09469					
A12	2.14439	-0.00010	0.00000	0.00006	0.00006
2.14445					
A13	2.12424	-0.00004	0.00000	-0.00465	-0.00466
2.11958					
A14	2.08725	-0.00001	0.00000	-0.00401	-0.00401
2.08325					
A15	2.07160	0.00005	0.00000	0.00868	0.00868
2.08028					
A16	2.10699	0.00002	0.00000	0.00395	0.00395
2.11095					
A17	2.08675	-0.00007	0.00000	-0.00677	-0.00677
2.07998					
A18	2.08944	0.00005	0.00000	0.00282	0.00281
2.09225					
A19	2.11917	-0.00001	0.00000	-0.00224	-0.00224
2.11693					
A20	2.08214	0.00001	0.00000	0.00129	0.00129
2.08343					
A21	2.08184	0.00000	0.00000	0.00096	0.00096
2.08280					
A22	2.08777	-0.00001	0.00000	0.00266	0.00266
2.09043					
A23	2.09053	-0.00034	0.00000	-0.00785	-0.00785
2.08267					
A24	2.10481	0.00035	0.00000	0.00519	0.00520
2.11001					
A25	2.09167	-0.00009	0.00000	-0.00191	-0.00191
2.08976					
A26	2.14939	0.00019	0.00000	0.00361	0.00362
2.15301					
A27	2.04209	-0.00010	0.00000	-0.00171	-0.00172
2.04037					
A28	2.08723	0.00004	0.00000	0.00175	0.00174
2.08897					
A29	2.11053	-0.00010	0.00000	-0.00737	-0.00737
2.10316					

This journal is © The Royal Society of Chemistry 2014

```
   A30        2.08542   0.00006   0.00000   0.00562   0.00562
2.09104
   A31        2.06285  -0.00009   0.00000  -0.00384  -0.00384
2.05900
   A32        2.11686   0.00000   0.00000  -0.00328  -0.00327
2.11358
   A33        2.10347   0.00009   0.00000   0.00711   0.00711
2.11058
   A34        2.08883  -0.00001   0.00000  -0.00162  -0.00161
2.08722
   A35        2.10193   0.00009   0.00000   0.00591   0.00591
2.10785
   A36        2.09241  -0.00009   0.00000  -0.00430  -0.00430
2.08811
   A37        2.10756   0.00005   0.00000   0.00460   0.00460
2.11216
   A38        2.08675  -0.00008   0.00000  -0.00655  -0.00655
2.08020
   A39        2.08887   0.00003   0.00000   0.00194   0.00194
2.09081
   A40        2.12545   0.00000   0.00000  -0.00362  -0.00362
2.12183
   A41        2.08891   0.00001   0.00000  -0.00256  -0.00255
2.08636
   A42        2.06871  -0.00001   0.00000   0.00618   0.00618
2.07489
   A43        1.95094  -0.00009   0.00000  -0.01118  -0.01123
1.93971
   A44        1.95674   0.00011   0.00000  -0.00353  -0.00355
1.95319
   A45        1.94724  -0.00001   0.00000  -0.01185  -0.01190
1.93534
   A46        1.87446  -0.00002   0.00000   0.00975   0.00974
1.88420
   A47        1.87235   0.00004   0.00000   0.01036   0.01029
1.88264
   A48        1.85684  -0.00003   0.00000   0.00866   0.00863
1.86547
    D1       -0.00087  -0.00002   0.00000   0.00086   0.00086  -
0.00001
    D2        3.13533  -0.00001   0.00000   0.00033   0.00033
3.13566
    D3       -3.13902   0.00000   0.00000   0.00001   0.00001  -
3.13901
    D4       -0.00282   0.00001   0.00000  -0.00052  -0.00052  -
0.00334
    D5        0.00864   0.00000   0.00000  -0.00108  -0.00109
0.00756
    D6       -3.13070   0.00001   0.00000   0.00002   0.00001  -
3.13068
    D7       -3.13638  -0.00001   0.00000  -0.00023  -0.00023  -
3.13661
```

D8	0.00747	-0.00001	0.00000	0.00087	0.00087	0.00834
D9	-0.01180	0.00000	0.00000	0.00052	0.00052	-0.01128
D10	3.12700	-0.00001	0.00000	-0.00013	-0.00013	3.12687
D11	3.13506	-0.00001	0.00000	0.00101	0.00101	3.13607
D12	-0.00932	-0.00002	0.00000	0.00035	0.00035	-0.00897
D13	0.01638	0.00003	0.00000	-0.00163	-0.00164	0.01474
D14	-3.13181	-0.00002	0.00000	-0.00011	-0.00011	-3.13192
D15	-3.12247	0.00004	0.00000	-0.00098	-0.00099	-3.12346
D16	0.01253	-0.00001	0.00000	0.00055	0.00054	0.01307
D17	-3.12400	0.00003	0.00000	0.00145	0.00145	-3.12255
D18	0.00818	0.00001	0.00000	0.00230	0.00230	0.01048
D19	0.01480	0.00002	0.00000	0.00081	0.00081	0.01561
D20	-3.13621	-0.00001	0.00000	0.00166	0.00166	-3.13455
D21	-0.00904	-0.00004	0.00000	0.00150	0.00150	-0.00754
D22	3.11774	-0.00003	0.00000	0.00284	0.00284	3.12057
D23	3.13935	0.00001	0.00000	-0.00007	-0.00007	3.13928
D24	-0.01706	0.00003	0.00000	0.00127	0.00126	-0.01580
D25	-0.04002	0.00000	0.00000	-0.00190	-0.00190	-0.04193
D26	3.11470	0.00004	0.00000	-0.00195	-0.00195	3.11274
D27	3.09458	-0.00006	0.00000	-0.00028	-0.00029	3.09429
D28	-0.03388	-0.00002	0.00000	-0.00034	-0.00034	-0.03422
D29	-0.00341	0.00002	0.00000	-0.00013	-0.00013	-0.00355
D30	3.13592	0.00002	0.00000	-0.00125	-0.00125	3.13467
D31	-3.13032	0.00001	0.00000	-0.00136	-0.00136	-3.13168
D32	0.00902	0.00001	0.00000	-0.00247	-0.00248	0.00654
D33	-0.01413	-0.00001	0.00000	-0.00095	-0.00095	-0.01508

D34	3.12377	-0.00002	0.00000	-0.00206	-0.00206	3.12172
D35	3.13688	0.00001	0.00000	-0.00180	-0.00180	3.13508
D36	-0.00840	0.00001	0.00000	-0.00291	-0.00291	-0.01131
D37	0.04064	0.00001	0.00000	0.00173	0.00173	0.04238
D38	-3.09148	0.00001	0.00000	0.00307	0.00308	-3.08840
D39	-3.11419	-0.00004	0.00000	0.00168	0.00168	-3.11251
D40	0.03687	-0.00004	0.00000	0.00302	0.00303	0.03990
D41	1.46924	-0.00005	0.00000	-0.00125	-0.00123	1.46802
D42	-2.70804	-0.00006	0.00000	0.00090	0.00090	-2.70714
D43	-0.62732	-0.00003	0.00000	0.00140	0.00138	-0.62593
D44	-1.65909	0.00000	0.00000	-0.00128	-0.00126	-1.66035
D45	0.44681	-0.00001	0.00000	0.00087	0.00087	0.44768
D46	2.52754	0.00002	0.00000	0.00137	0.00135	2.52889
D47	-0.01387	0.00000	0.00000	-0.00030	-0.00030	-0.01418
D48	3.13135	0.00001	0.00000	0.00083	0.00083	3.13218
D49	3.11882	0.00000	0.00000	-0.00153	-0.00153	3.11729
D50	-0.01914	0.00000	0.00000	-0.00041	-0.00040	-0.01954
D51	-3.13941	0.00000	0.00000	-0.00094	-0.00094	-3.14035
D52	0.01841	-0.00002	0.00000	-0.00136	-0.00136	0.01705
D53	0.01140	0.00001	0.00000	0.00037	0.00037	0.01177
D54	-3.11397	-0.00001	0.00000	-0.00005	-0.00005	-3.11401
D55	0.01120	0.00001	0.00000	0.00040	0.00040	0.01160
D56	-3.12469	-0.00001	0.00000	0.00151	0.00150	-3.12319
D57	-3.13407	0.00000	0.00000	-0.00073	-0.00072	-3.13480
D58	0.01322	-0.00001	0.00000	0.00038	0.00038	0.01360
D59	0.00137	0.00001	0.00000	-0.00035	-0.00035	0.00103

```
   D60        3.13847   0.00001   0.00000  -0.00010  -0.00009
3.13837
   D61       -3.13439   0.00000   0.00000   0.00083   0.00083  -
3.13356
   D62        0.00271   0.00000   0.00000   0.00108   0.00108
0.00379
   D63       -0.00962   0.00001   0.00000   0.00036   0.00037  -
0.00925
   D64        3.12919   0.00001   0.00000  -0.00109  -0.00109
3.12810
   D65        3.13645   0.00001   0.00000   0.00009   0.00009
3.13654
   D66       -0.00793   0.00001   0.00000  -0.00137  -0.00137  -
0.00929
   D67        0.00289  -0.00002   0.00000  -0.00040  -0.00040
0.00249
   D68        3.12844   0.00001   0.00000  -0.00006  -0.00006
3.12837
   D69       -3.13592  -0.00002   0.00000   0.00108   0.00108  -
3.13484
   D70       -0.01038   0.00001   0.00000   0.00142   0.00142  -
0.00896
         Item               Value     Threshold  Converged?
 Maximum Force            0.000346     0.000450     YES
 RMS     Force            0.000068     0.000300     YES
 Maximum Displacement     0.041386     0.001800     NO
 RMS     Displacement     0.006776     0.001200     NO
 Predicted change in Energy=-2.353104D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.787915   -5.430483    0.011762
      2          6           0       -3.422889   -5.397677   -0.017418
      3          6           0       -2.712805   -4.150612   -0.030196
      4          6           0       -3.446984   -2.907614   -0.026178
      5          6           0       -4.883161   -2.994170    0.009703
      6          6           0       -5.526131   -4.204230    0.029985
      7          6           0       -1.312315   -4.123173   -0.042422
      8          6           0       -2.750461   -1.671826   -0.050638
      9          6           0       -1.334944   -1.662097   -0.027437
     10          6           0       -0.608722   -2.913068   -0.032168
     11          6           0        0.826996   -2.904916   -0.020386
     12          1           0        1.342766   -3.862607   -0.030867
     13          6           0        1.525250   -1.732276    0.011198
     14          6           0        0.816883   -0.487907    0.034282
     15          6           0       -0.552245   -0.454667    0.014317
```

16	1	0	-0.760260	-5.060693	-0.052117
17	1	0	-5.320210	-6.377452	0.023734
18	1	0	-2.841737	-6.317194	-0.026134
19	1	0	-5.470528	-2.082467	0.033717
20	1	0	-6.610880	-4.239875	0.063499
21	1	0	2.611545	-1.732405	0.022977
22	1	0	1.378618	0.440529	0.072142
23	1	0	-1.053660	0.507087	0.045425
24	6	0	-3.536234	-0.378295	-0.084102
25	1	0	-3.836923	-0.071296	0.926635
26	1	0	-2.960901	0.435926	-0.525516
27	1	0	-4.443581	-0.488556	-0.685281

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.365731	0.000000			
3	C	2.438423	1.435114	0.000000		
4	C	2.857341	2.490195	1.443635	0.000000	
5	C	2.438174	2.812468	2.459552	1.439230	0.000000
6	C	1.431430	2.418716	2.814481	2.450963	1.370426
7	C	3.713730	2.465666	1.400812	2.456555	3.745438
8	C	4.275817	3.786189	2.479156	1.418772	2.510108
9	C	5.111289	4.279506	2.844506	2.451944	3.790203
10	C	4.879033	3.754069	2.441042	2.838274	4.275414
11	C	6.156845	4.927006	3.752605	4.273985	5.710933
12	H	6.328136	5.006805	4.065785	4.884030	6.286334
13	C	7.316610	6.157927	4.879669	5.109396	6.531470
14	C	7.472839	6.487232	5.087069	4.902979	6.226754
15	C	6.534496	5.716201	4.281356	3.794483	5.020550
16	H	4.045099	2.684093	2.154335	3.443096	4.612228
17	H	1.086385	2.135762	3.429327	3.943506	3.411423
18	H	2.138995	1.087808	2.170418	3.462883	3.900152
19	H	3.416965	3.896929	3.447658	2.186135	1.084795
20	H	2.177940	3.392689	3.900222	3.434122	2.130654
21	H	8.272116	7.060471	5.848013	6.171654	7.600187
22	H	8.514607	7.559572	6.150511	5.874194	7.142193
23	H	7.014309	6.362660	4.944962	4.170529	5.188946
24	C	5.205814	5.021105	3.861518	2.531556	2.943776
25	H	5.519262	5.425218	4.338201	3.017383	3.237062
26	H	6.167771	5.873885	4.619873	3.415388	3.968262
27	H	5.002706	5.058391	4.103094	2.698048	2.637107

		6	7	8	9	10
6	C	0.000000				
7	C	4.215218	0.000000			
8	C	3.758180	2.842083	0.000000		
9	C	4.902223	2.461226	1.415741	0.000000	
10	C	5.084474	1.399823	2.475494	1.446495	0.000000
11	C	6.484827	2.461968	3.784128	2.493718	1.435789
12	H	6.877657	2.667861	4.642674	3.465889	2.170238
13	C	7.472141	3.710935	4.276585	2.861315	2.439259
14	C	7.351524	4.213613	3.759630	2.452120	2.813925

This journal is © The Royal Society of Chemistry 2014

15	C	6.228885	3.746847	2.513533	1.439531	2.459489
16	H	4.842912	1.088026	3.930053	3.446929	2.153057
17	H	2.182965	4.598845	5.362094	6.174102	5.848350
18	H	3.416685	2.674532	4.646329	4.892888	4.071175
19	H	2.122495	4.632604	2.752183	4.157344	4.932687
20	H	1.085851	5.300908	4.637967	5.872709	6.147802
21	H	8.504807	4.595294	5.362853	3.947437	3.430324
22	H	8.321726	5.299209	4.639656	3.434293	3.899617
23	H	6.496134	4.638312	2.763336	2.188559	3.449849
24	C	4.313988	4.355648	1.513864	2.548929	3.872738
25	H	4.553960	4.871389	2.167293	3.114611	4.406388
26	H	5.331045	4.872023	2.170810	2.700653	4.122124
27	H	3.935702	4.840304	2.160915	3.387268	4.583772

		11	12	13	14	15
11	C	0.000000				
12	H	1.087796	0.000000			
13	C	1.365153	2.138547	0.000000		
14	C	2.417649	3.416050	1.432051	0.000000	
15	C	2.811980	3.899637	2.438909	1.369677	0.000000
16	H	2.677267	2.420450	4.038059	4.837894	4.611199
17	H	7.060353	7.121986	8.272735	8.505925	7.603483
18	H	5.010317	4.851297	6.331938	6.882568	6.293857
19	H	6.351233	7.042305	7.004573	6.486460	5.180697
20	H	7.557192	7.963148	8.513953	8.321645	7.144037
21	H	2.135715	2.480012	1.086359	2.183968	3.412075
22	H	3.391880	4.304518	2.178599	1.085804	2.129073
23	H	3.896532	4.984266	3.415654	2.118742	1.085060
24	C	5.042385	5.995657	5.240320	4.356105	2.986587
25	H	5.538808	6.489995	5.687686	4.756866	3.430511
26	H	5.075879	6.102755	5.011458	3.929185	2.624157
27	H	5.836083	6.730104	6.136682	5.309450	3.953869

		16	17	18	19	20
16	H	0.000000				
17	H	4.746868	0.000000			
18	H	2.431464	2.479707	0.000000		
19	H	5.573493	4.297627	4.984681	0.000000	
20	H	5.909049	2.497328	4.304617	2.440430	0.000000
21	H	4.738376	9.191801	7.124675	8.089658	9.557310
22	H	5.903700	9.558321	7.967927	7.299163	9.259499
23	H	5.576358	8.099433	7.055009	5.120025	7.308671
24	C	5.443519	6.259720	5.979650	2.580616	4.938324
25	H	5.942886	6.540870	6.396046	2.740579	5.081032
26	H	5.939675	7.231192	6.772608	3.599066	5.960906
27	H	5.905267	5.995855	6.080576	2.027839	4.396618

		21	22	23	24	25
21	H	0.000000				
22	H	2.498833	0.000000			
23	H	4.295295	2.433335	0.000000		
24	C	6.296051	4.985042	2.638911	0.000000	
25	H	6.720017	5.309801	2.976175	1.098295	0.000000
26	H	6.004553	4.380484	1.992137	1.090325	1.770150
27	H	7.198861	5.944316	3.607881	1.094008	1.772121

```
                    26         27
    26  H    0.000000
    27  H    1.754574   0.000000
 Stoichiometry    C15H12
 Framework group  C1[X(C15H12)]
 Deg. of freedom    75
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.654795   -1.005467    0.022716
      2          6           0       -2.459598   -1.665533   -0.009527
      3          6           0       -1.217444   -0.946851   -0.019622
      4          6           0       -1.224414    0.496732   -0.009574
      5          6           0       -2.508157    1.146246    0.029348
      6          6           0       -3.673694    0.425633    0.046919
      7          6           0        0.005673   -1.629510   -0.035012
      8          6           0        0.000340    1.212565   -0.031360
      9          6           0        1.227509    0.506887   -0.011419
     10          6           0        1.223585   -0.939563   -0.022189
     11          6           0        2.467398   -1.656744   -0.013721
     12          1           0        2.429686   -2.743783   -0.028731
     13          6           0        3.661809   -0.996543    0.020314
     14          6           0        3.677824    0.435124    0.049372
     15          6           0        2.512385    1.154492    0.032709
     16          1           0        0.009466   -2.717436   -0.049251
     17          1           0       -4.592066   -1.554702    0.032634
     18          1           0       -2.421600   -2.752596   -0.022792
     19          1           0       -2.555460    2.229633    0.057898
     20          1           0       -4.628311    0.941858    0.082834
     21          1           0        4.599729   -1.544627    0.029564
     22          1           0        4.631179    0.953297    0.089152
     23          1           0        2.564548    2.237713    0.068327
     24          6           0       -0.025699    2.725961   -0.058498
     25          1           0       -0.130225    3.138490    0.953997
     26          1           0        0.881664    3.140658   -0.498417
     27          1           0       -0.864935    3.090928   -0.657943
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3917273      0.4478742
0.3396564
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
```

```
      nuclear repulsion energy       878.7188367632 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
```

This journal is © The Royal Society of Chemistry 2014

```
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860335407     A.U. after   12 cycles
            Convg  =    0.4708D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.005297124    0.003749976    0.000034579
      2        6           0.003985615    0.002736180   -0.000009076
      3        6           0.002706903   -0.002924926    0.000122428
      4        6          -0.001730188    0.000502171   -0.000289190
      5        6           0.003684956    0.001250250   -0.000016713
      6        6           0.001005810   -0.004765819    0.000082579
      7        6          -0.001686721    0.002422368   -0.000078038
      8        6          -0.001400898   -0.000906783   -0.000285751
      9        6           0.001693007    0.000992505    0.000163173
     10        6           0.001504052   -0.003442554    0.000084601
     11        6          -0.004363503   -0.002049182   -0.000030272
     12        1           0.000260414    0.000086089   -0.000037661
     13        6          -0.000886650    0.006610049    0.000059115
     14        6           0.004012270   -0.003367149    0.000035142
     15        6          -0.003235635   -0.001710472   -0.000177943
     16        1           0.000103398   -0.000200357    0.000083067
     17        1          -0.000099700   -0.000331372    0.000039727
     18        1          -0.000197588   -0.000177105   -0.000036369
     19        1          -0.000397810   -0.000957942    0.000172491
     20        1          -0.000940115    0.000184136   -0.000046276
     21        1           0.000333041   -0.000054913    0.000029916
     22        1           0.000363511    0.000902560   -0.000022242
     23        1           0.000580307   -0.000410106   -0.000039892
     24        6           0.000669501   -0.002134619   -0.000325046
     25        1          -0.000825514    0.001249926   -0.000038112
     26        1          -0.000194916    0.001133091   -0.000017884
     27        1           0.000353574    0.001613999    0.000543645
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.006610049 RMS     0.001850562


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.004364457 RMS     0.000948319
 Search for a local minimum.
 Step number  23 out of a maximum of  157
```

This journal is © The Royal Society of Chemistry 2014

```
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
21
                                                     20   22   23
 DE=  2.39D-04 DEPred=-2.35D-04 R=-1.02D+00
 Trust test=-1.02D+00 RLast= 5.03D-02 DXMaxT set to 5.00D-02
     Eigenvalues ---   -0.00351   0.00000   0.01273   0.01715
0.01766
     Eigenvalues ---    0.01813   0.01819   0.01840   0.01944
0.01976
     Eigenvalues ---    0.01990   0.02001   0.02040   0.02101
0.02112
     Eigenvalues ---    0.02136   0.02149   0.02213   0.02228
0.02250
     Eigenvalues ---    0.02349   0.02358   0.06436   0.06839
0.08870
     Eigenvalues ---    0.14694   0.15740   0.15854   0.15924
0.16000
     Eigenvalues ---    0.16000   0.16001   0.16003   0.16065
0.16247
     Eigenvalues ---    0.16309   0.21471   0.21956   0.22033
0.22599
     Eigenvalues ---    0.23305   0.23847   0.24461   0.24992
0.25461
     Eigenvalues ---    0.27128   0.30308   0.32260   0.33255
0.33600
     Eigenvalues ---    0.33631   0.33651   0.33682   0.33682
0.33806
     Eigenvalues ---    0.33988   0.34439   0.35871   0.36368
0.37136
     Eigenvalues ---    0.37280   0.38218   0.38891   0.39610
0.40335
     Eigenvalues ---    0.41121   0.42127   0.44468   0.45519
0.47136
     Eigenvalues ---    0.49274   0.49408   0.49876   0.51323
0.96674
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is  -3.51D-03 should be greater than     0.000000
Eigenvector:
                          D28       D27       D40       D39       D26
   1                    0.31154   0.28499  -0.27478  -0.25743
0.25452
                          D38       D37       D25       D41       D42
   1                   -0.24646  -0.22911   0.22797  -0.16834  -
0.16563
 Eigenvalue     2 is   7.49D-07 Eigenvector:
                          D44       D46       D45       D41       D43
   1                    0.40080   0.39904   0.38251   0.38185
0.38009
                          D42       D28       D40       D27       D39
   1                    0.36356   0.11895  -0.10252   0.10018  -
0.09978
 Use linear search instead of GDIIS.
 RFO step:  Lambda=-2.77131151D-05 EMin= 3.51158919D-03
 Quartic linear search produced a step of -0.96102.
 Maximum step size (   0.050) exceeded in Quadratic search.
    -- Step size scaled by   0.137
 Iteration  1 RMS(Cart)=  0.00825930 RMS(Int)=  0.00007863
 Iteration  2 RMS(Cart)=  0.00008263 RMS(Int)=  0.00000229
 Iteration  3 RMS(Cart)=  0.00000001 RMS(Int)=  0.00000229
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58086   0.00356   0.00874   0.00011   0.00885
2.58971
    R2        2.70501  -0.00430  -0.01294   0.00004  -0.01290
2.69211
```

R3	2.05297	0.00034	0.00103	-0.00008	0.00095
2.05392					
R4	2.71197	-0.00192	-0.00716	-0.00006	-0.00723
2.70475					
R5	2.05566	0.00005	0.00035	-0.00012	0.00023
2.05589					
R6	2.72807	0.00113	0.00625	-0.00019	0.00607
2.73414					
R7	2.64715	-0.00183	-0.00487	0.00022	-0.00465
2.64250					
R8	2.71975	-0.00147	-0.00754	-0.00015	-0.00769
2.71206					
R9	2.68109	0.00003	-0.00155	0.00016	-0.00140
2.67969					
R10	2.58973	0.00143	0.00514	0.00012	0.00526
2.59499					
R11	2.04997	-0.00059	-0.00096	0.00003	-0.00093
2.04904					
R12	2.05196	0.00093	0.00248	-0.00015	0.00232
2.05428					
R13	2.64528	-0.00187	-0.00348	-0.00001	-0.00349
2.64179					
R14	2.05607	0.00022	0.00103	-0.00010	0.00092
2.05699					
R15	2.67536	0.00051	0.00350	-0.00049	0.00301
2.67837					
R16	2.86079	0.00159	0.00090	-0.00005	0.00086
2.86165					
R17	2.73348	0.00017	0.00338	0.00036	0.00375
2.73723					
R18	2.72032	-0.00148	-0.00726	-0.00010	-0.00736
2.71296					
R19	2.71325	-0.00193	-0.00793	0.00011	-0.00783
2.70542					
R20	2.05564	0.00005	0.00035	-0.00012	0.00023
2.05587					
R21	2.57976	0.00376	0.00923	-0.00002	0.00922
2.58898					
R22	2.70618	-0.00436	-0.01392	0.00019	-0.01373
2.69246					
R23	2.05292	0.00033	0.00106	-0.00008	0.00098
2.05390					
R24	2.58832	0.00163	0.00598	-0.00005	0.00593
2.59424					
R25	2.05187	0.00096	0.00255	-0.00016	0.00239
2.05427					
R26	2.05047	-0.00063	-0.00179	0.00009	-0.00170
2.04877					
R27	2.07548	0.00054	0.00215	0.00006	0.00221
2.07768					
R28	2.06042	0.00075	0.00258	-0.00025	0.00233
2.06275					

This journal is © The Royal Society of Chemistry 2014

R29	2.06738	-0.00075	-0.00114	0.00053	-0.00062
2.06676					
A1	2.08880	0.00004	0.00075	0.00023	0.00098
2.08978					
A2	2.10702	-0.00010	-0.00529	-0.00050	-0.00579
2.10123					
A3	2.08737	0.00006	0.00453	0.00027	0.00480
2.09217					
A4	2.11250	0.00062	0.00364	-0.00012	0.00352
2.11602					
A5	2.11044	-0.00058	-0.00670	-0.00036	-0.00705
2.10339					
A6	2.06022	-0.00004	0.00306	0.00048	0.00354
2.06376					
A7	2.09040	-0.00100	-0.00535	-0.00022	-0.00557
2.08484					
A8	2.10805	0.00053	0.00483	0.00046	0.00528
2.11333					
A9	2.08473	0.00047	0.00052	-0.00024	0.00028
2.08501					
A10	2.04404	-0.00011	0.00026	0.00049	0.00075
2.04479					
A11	2.09469	-0.00033	-0.00021	0.00018	-0.00003
2.09466					
A12	2.14445	0.00044	-0.00006	-0.00068	-0.00074
2.14371					
A13	2.11958	0.00109	0.00447	-0.00028	0.00419
2.12378					
A14	2.08325	0.00034	0.00385	-0.00020	0.00365
2.08689					
A15	2.08028	-0.00142	-0.00834	0.00048	-0.00786
2.07241					
A16	2.11095	-0.00064	-0.00380	-0.00013	-0.00393
2.10702					
A17	2.07998	0.00054	0.00651	0.00020	0.00671
2.08670					
A18	2.09225	0.00010	-0.00270	-0.00008	-0.00278
2.08947					
A19	2.11693	0.00038	0.00215	-0.00005	0.00211
2.11903					
A20	2.08343	-0.00020	-0.00124	0.00007	-0.00116
2.08227					
A21	2.08280	-0.00018	-0.00092	-0.00003	-0.00095
2.08185					
A22	2.09043	-0.00099	-0.00256	0.00010	-0.00245
2.08798					
A23	2.08267	0.00258	0.00755	-0.00139	0.00616
2.08883					
A24	2.11001	-0.00159	-0.00499	0.00129	-0.00370
2.10631					
A25	2.08976	0.00063	0.00183	-0.00028	0.00155
2.09131					

This journal is © The Royal Society of Chemistry 2014

A26	2.15301	-0.00109	-0.00348	0.00011	-0.00336	2.14964
A27	2.04037	0.00046	0.00165	0.00017	0.00182	2.04219
A28	2.08897	-0.00017	-0.00168	0.00017	-0.00151	2.08746
A29	2.10316	0.00135	0.00708	0.00002	0.00710	2.11026
A30	2.09104	-0.00118	-0.00540	-0.00019	-0.00559	2.08546
A31	2.05900	0.00000	0.00369	0.00031	0.00400	2.06300
A32	2.11358	0.00055	0.00314	-0.00001	0.00313	2.11672
A33	2.11058	-0.00055	-0.00683	-0.00030	-0.00713	2.10345
A34	2.08722	0.00021	0.00155	0.00008	0.00163	2.08885
A35	2.10785	-0.00016	-0.00568	-0.00040	-0.00608	2.10176
A36	2.08811	-0.00005	0.00413	0.00032	0.00445	2.09257
A37	2.11216	-0.00088	-0.00442	0.00000	-0.00442	2.10774
A38	2.08020	0.00060	0.00629	0.00025	0.00655	2.08675
A39	2.09081	0.00028	-0.00187	-0.00026	-0.00212	2.08869
A40	2.12183	0.00083	0.00348	-0.00007	0.00341	2.12524
A41	2.08636	-0.00008	0.00245	-0.00003	0.00242	2.08878
A42	2.07489	-0.00074	-0.00594	0.00009	-0.00585	2.06904
A43	1.93971	0.00146	0.01079	0.00025	0.01105	1.95076
A44	1.95319	0.00045	0.00341	0.00011	0.00353	1.95672
A45	1.93534	0.00178	0.01144	-0.00180	0.00965	1.94499
A46	1.88420	-0.00122	-0.00936	0.00050	-0.00886	1.87534
A47	1.88264	-0.00146	-0.00989	0.00040	-0.00947	1.87317
A48	1.86547	-0.00125	-0.00830	0.00061	-0.00768	1.85779
D1	-0.00001	-0.00005	-0.00082	-0.00023	-0.00105	-0.00106
D2	3.13566	-0.00004	-0.00031	-0.00050	-0.00082	3.13484
D3	-3.13901	0.00001	-0.00001	0.00018	0.00017	-3.13883

D4	-0.00334	0.00002	0.00050	-0.00009	0.00041	-0.00293
D5	0.00756	0.00005	0.00104	0.00075	0.00180	0.00935
D6	-3.13068	0.00003	-0.00001	0.00108	0.00107	-3.12962
D7	-3.13661	-0.00001	0.00022	0.00035	0.00057	-3.13604
D8	0.00834	-0.00003	-0.00084	0.00067	-0.00016	0.00818
D9	-0.01128	-0.00003	-0.00050	-0.00088	-0.00138	-0.01266
D10	3.12687	-0.00006	0.00013	-0.00116	-0.00103	3.12583
D11	3.13607	-0.00004	-0.00097	-0.00060	-0.00157	3.13450
D12	-0.00897	-0.00006	-0.00034	-0.00089	-0.00123	-0.01019
D13	0.01474	0.00010	0.00157	0.00143	0.00300	0.01774
D14	-3.13192	-0.00003	0.00011	0.00010	0.00021	-3.13171
D15	-3.12346	0.00013	0.00095	0.00170	0.00265	-3.12080
D16	0.01307	-0.00001	-0.00052	0.00038	-0.00014	0.01293
D17	-3.12255	0.00005	-0.00139	0.00171	0.00032	-3.12223
D18	0.01048	-0.00001	-0.00221	0.00149	-0.00072	0.00976
D19	0.01561	0.00002	-0.00077	0.00143	0.00065	0.01626
D20	-3.13455	-0.00004	-0.00159	0.00121	-0.00039	-3.13493
D21	-0.00754	-0.00011	-0.00144	-0.00093	-0.00238	-0.00992
D22	3.12057	-0.00015	-0.00273	-0.00157	-0.00430	3.11627
D23	3.13928	0.00003	0.00007	0.00043	0.00050	3.13978
D24	-0.01580	-0.00001	-0.00121	-0.00021	-0.00142	-0.01722
D25	-0.04193	0.00004	0.00183	-0.00246	-0.00063	-0.04256
D26	3.11274	0.00010	0.00188	-0.00274	-0.00087	3.11188
D27	3.09429	-0.00011	0.00028	-0.00386	-0.00358	3.09071
D28	-0.03422	-0.00004	0.00032	-0.00415	-0.00382	-0.03804
D29	-0.00355	0.00003	0.00013	-0.00015	-0.00002	-0.00357

This journal is © The Royal Society of Chemistry 2014

D30	3.13467	0.00005	0.00120	-0.00048	0.00073	3.13540
D31	-3.13168	0.00006	0.00131	0.00050	0.00180	-3.12988
D32	0.00654	0.00008	0.00238	0.00017	0.00255	0.00909
D33	-0.01508	-0.00002	0.00091	-0.00113	-0.00023	-0.01531
D34	3.12172	-0.00001	0.00197	-0.00132	0.00065	3.12237
D35	3.13508	0.00004	0.00173	-0.00092	0.00081	3.13589
D36	-0.01131	0.00006	0.00280	-0.00110	0.00169	-0.00962
D37	0.04238	-0.00002	-0.00166	0.00274	0.00108	0.04345
D38	-3.08840	-0.00008	-0.00296	0.00277	-0.00019	-3.08860
D39	-3.11251	-0.00005	-0.00162	0.00301	0.00139	-3.11111
D40	0.03990	-0.00011	-0.00291	0.00303	0.00013	0.04002
D41	1.46802	0.00001	0.00118	-0.02021	-0.01904	1.44898
D42	-2.70714	-0.00022	-0.00086	-0.01932	-0.02018	-2.72732
D43	-0.62593	-0.00030	-0.00133	-0.01969	-0.02101	-0.64694
D44	-1.66035	0.00007	0.00121	-0.02049	-0.01929	-1.67963
D45	0.44768	-0.00016	-0.00084	-0.01960	-0.02043	0.42725
D46	2.52889	-0.00024	-0.00130	-0.01996	-0.02126	2.50763
D47	-0.01418	0.00000	0.00029	-0.00097	-0.00068	-0.01486
D48	3.13218	-0.00002	-0.00080	-0.00079	-0.00159	3.13059
D49	3.11729	0.00005	0.00147	-0.00100	0.00047	3.11776
D50	-0.01954	0.00003	0.00039	-0.00082	-0.00043	-0.01997
D51	-3.14035	0.00005	0.00091	0.00035	0.00126	-3.13909
D52	0.01705	0.00003	0.00131	0.00080	0.00211	0.01916
D53	0.01177	-0.00001	-0.00035	0.00038	0.00002	0.01179
D54	-3.11401	-0.00004	0.00005	0.00083	0.00088	-3.11314
D55	0.01160	0.00000	-0.00038	0.00060	0.00022	0.01182

```
   D56       -3.12319  -0.00004  -0.00144   0.00078  -0.00066  -
3.12385
   D57       -3.13480   0.00002   0.00069   0.00042   0.00111  -
3.13368
   D58        0.01360  -0.00002  -0.00037   0.00060   0.00023
0.01383
   D59        0.00103   0.00001   0.00033   0.00009   0.00043
0.00145
   D60        3.13837   0.00001   0.00009   0.00003   0.00012
3.13849
   D61       -3.13356  -0.00003  -0.00080   0.00028  -0.00052  -
3.13408
   D62        0.00379  -0.00003  -0.00104   0.00021  -0.00083
0.00296
   D63       -0.00925   0.00000  -0.00035  -0.00056  -0.00091  -
0.01016
   D64        3.12810   0.00004   0.00105  -0.00084   0.00021
3.12831
   D65        3.13654  -0.00001  -0.00009  -0.00049  -0.00058
3.13596
   D66       -0.00929   0.00003   0.00131  -0.00077   0.00054  -
0.00875
   D67        0.00249   0.00001   0.00038   0.00031   0.00069
0.00318
   D68        3.12837   0.00004   0.00006  -0.00014  -0.00008
3.12829
   D69       -3.13484  -0.00003  -0.00104   0.00059  -0.00045  -
3.13529
   D70       -0.00896   0.00000  -0.00136   0.00014  -0.00122  -
0.01018
         Item               Value     Threshold  Converged?
 Maximum Force            0.004364     0.000450     NO
 RMS     Force            0.000948     0.000300     NO
 Maximum Displacement     0.040815     0.001800     NO
 RMS     Displacement     0.008265     0.001200     NO
 Predicted change in Energy=-2.429918D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792585   -5.428155    0.012348
      2          6           0       -3.422873   -5.396516   -0.018049
      3          6           0       -2.709143   -4.155942   -0.030609
      4          6           0       -3.446339   -2.910997   -0.026820
      5          6           0       -4.878337   -2.997774    0.012299
      6          6           0       -5.527276   -4.207793    0.033278
      7          6           0       -1.311136   -4.127396   -0.042769
```

8	6	0	-2.751513	-1.675102	-0.051279
9	6	0	-1.334410	-1.667275	-0.026953
10	6	0	-0.606917	-2.919799	-0.031974
11	6	0	0.824593	-2.903354	-0.020992
12	1	0	1.349794	-3.856030	-0.032606
13	6	0	1.522209	-1.724655	0.010395
14	6	0	0.816149	-0.487353	0.034477
15	6	0	-0.556280	-0.461522	0.014620
16	1	0	-0.759146	-5.065525	-0.051914
17	1	0	-5.320525	-6.378139	0.024141
18	1	0	-2.849044	-6.320751	-0.027960
19	1	0	-5.468923	-2.088854	0.040343
20	1	0	-6.613407	-4.236254	0.068696
21	1	0	2.609023	-1.728485	0.021274
22	1	0	1.371489	0.446413	0.071919
23	1	0	-1.056905	0.499598	0.046715
24	6	0	-3.530934	-0.377242	-0.086211
25	1	0	-3.853397	-0.068073	0.918403
26	1	0	-2.946246	0.441918	-0.508845
27	1	0	-4.429352	-0.466958	-0.703411

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370415	0.000000			
3	C	2.441537	1.431291	0.000000		
4	C	2.854819	2.485645	1.446845	0.000000	
5	C	2.431893	2.805933	2.459390	1.435158	0.000000
6	C	1.424602	2.417480	2.819334	2.452670	1.373211
7	C	3.716921	2.463881	1.398351	2.457432	3.742193
8	C	4.272637	3.781633	2.481287	1.418033	2.505372
9	C	5.109280	4.274225	2.843126	2.450937	3.785656
10	C	4.879921	3.750190	2.438730	2.839440	4.272361
11	C	6.158605	4.925122	3.749180	4.270942	5.703809
12	H	6.340538	5.015143	4.070002	4.888355	6.287149
13	C	7.320692	6.159318	4.880284	5.108352	6.525935
14	C	7.474617	6.486289	5.088267	4.903734	6.223333
15	C	6.527919	5.707240	4.276167	3.788679	5.011264
16	H	4.050217	2.684426	2.151809	3.444361	4.609496
17	H	1.086890	2.136925	3.429355	3.941604	3.409184
18	H	2.139090	1.087929	2.169327	3.461674	3.893819
19	H	3.407220	3.889776	3.448808	2.184326	1.084304
20	H	2.176969	3.396062	3.906353	3.434494	2.132482
21	H	8.274747	7.059728	5.846206	6.169932	7.594191
22	H	8.515274	7.558691	6.151726	5.873110	7.136267
23	H	7.006763	6.353436	4.940639	4.164968	5.180361
24	C	5.207034	5.020900	3.867429	2.535863	2.948286
25	H	5.516656	5.427209	4.349783	3.023469	3.233369
26	H	6.175627	5.878381	4.628741	3.424103	3.979453
27	H	5.025706	5.077722	4.125577	2.719820	2.668119

		6	7	8	9	10
6	C	0.000000				

This journal is © The Royal Society of Chemistry 2014

7	C	4.217593	0.000000			
8	C	3.758528	2.844029	0.000000		
9	C	4.902855	2.460282	1.417333	0.000000	
10	C	5.086563	1.397974	2.479704	1.448478	0.000000
11	C	6.484654	2.461725	3.781276	2.487814	1.431646
12	H	6.886376	2.674750	4.645160	3.463471	2.169159
13	C	7.474071	3.715351	4.274453	2.857439	2.441995
14	C	7.353959	4.216778	3.761158	2.453750	2.818923
15	C	6.224605	3.743225	2.509217	1.435637	2.459240
16	H	4.845413	1.088513	3.932492	3.446687	2.151211
17	H	2.180190	4.598426	5.359484	6.171221	5.846483
18	H	3.411931	2.678841	4.646731	4.893768	4.073527
19	H	2.119754	4.631389	2.750256	4.156496	4.933032
20	H	1.087081	5.304560	4.635528	5.871679	6.149887
21	H	8.505673	4.596359	5.361292	3.944203	3.429918
22	H	8.322024	5.303711	4.638442	3.435016	3.905927
23	H	6.491835	4.634837	2.758735	2.185811	3.449776
24	C	4.321202	4.358101	1.514318	2.548022	3.875230
25	H	4.552208	4.885187	2.176460	3.129927	4.424386
26	H	5.345599	4.875392	2.174641	2.697950	4.123228
27	H	3.967618	4.853713	2.167956	3.387776	4.591108

		11	12	13	14	15
11	C	0.000000				
12	H	1.087917	0.000000			
13	C	1.370031	2.138770	0.000000		
14	C	2.416652	3.411343	1.424787	0.000000	
15	C	2.805462	3.893332	2.432208	1.372815	0.000000
16	H	2.680329	2.431230	4.045970	4.842383	4.608950
17	H	7.059649	7.131439	8.275150	8.506482	7.596347
18	H	5.017395	4.868789	6.342982	6.889562	6.291991
19	H	6.346300	7.044370	7.000676	6.485906	5.175224
20	H	7.557017	7.972917	8.514680	8.321883	7.137249
21	H	2.136889	2.472854	1.086876	2.180592	3.409454
22	H	3.395389	4.303767	2.177162	1.087071	2.131647
23	H	3.889048	4.976945	3.405942	2.117203	1.084162
24	C	5.035485	5.993859	5.230593	4.350151	2.977556
25	H	5.550214	6.505862	5.697884	4.770931	3.441310
26	H	5.064393	6.095501	4.993069	3.913357	2.608095
27	H	5.831437	6.733077	6.124737	5.297186	3.939072

		16	17	18	19	20
16	H	0.000000				
17	H	4.747096	0.000000			
18	H	2.437999	2.472697	0.000000		
19	H	5.572350	4.291882	4.977689	0.000000	
20	H	5.913933	2.502238	4.304056	2.433511	0.000000
21	H	4.741914	9.192226	7.133150	8.086003	9.557425
22	H	5.910701	9.558234	7.976050	7.295191	9.256670
23	H	5.573955	8.092109	7.052269	5.115274	7.300924
24	C	5.446465	6.263033	5.982781	2.588713	4.941418
25	H	5.957385	6.539809	6.403149	2.732118	5.070837
26	H	5.943410	7.241164	6.780442	3.615289	5.972179
27	H	5.919601	6.022091	6.100861	2.065049	4.424233

This journal is © The Royal Society of Chemistry 2014

		21	22	23	24	25
21	H	0.000000				
22	H	2.502846	0.000000			
23	H	4.289991	2.429107	0.000000		
24	C	6.287804	4.973647	2.628181	0.000000	
25	H	6.732361	5.317957	2.983699	1.099462	0.000000
26	H	5.987712	4.356621	1.970174	1.091559	1.766366
27	H	7.187165	5.923271	3.587523	1.093682	1.766667

		26	27
26	H	0.000000	
27	H	1.750290	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.657850	-0.996817	0.022308
2	6	0	-2.459746	-1.661262	-0.010769
3	6	0	-1.217115	-0.951073	-0.020389
4	6	0	-1.224491	0.495720	-0.010687
5	6	0	-2.504203	1.144007	0.031043
6	6	0	-3.675482	0.427425	0.049058
7	6	0	0.003846	-1.632555	-0.035297
8	6	0	-0.000538	1.211469	-0.032185
9	6	0	1.226437	0.502312	-0.010719
10	6	0	1.221609	-0.946117	-0.021659
11	6	0	2.465371	-1.655060	-0.013538
12	1	0	2.437419	-2.742499	-0.029597
13	6	0	3.662838	-0.990311	0.020603
14	6	0	3.678474	0.434076	0.050506
15	6	0	2.507057	1.149698	0.033538
16	1	0	0.006362	-2.720981	-0.048890
17	1	0	-4.593351	-1.550060	0.031812
18	1	0	-2.431364	-2.748726	-0.025123
19	1	0	-2.554784	2.226643	0.063510
20	1	0	-4.627238	0.951349	0.086589
21	1	0	4.598872	-1.542638	0.029253
22	1	0	4.629428	0.959281	0.090124
23	1	0	2.560483	2.231926	0.070058
24	6	0	-0.017625	2.725418	-0.060930
25	1	0	-0.139786	3.151021	0.945427
26	1	0	0.900780	3.138770	-0.481851
27	1	0	-0.838300	3.104326	-0.676612

Rotational constants (GHZ): 1.3934064 0.4479389
0.3397957

This journal is © The Royal Society of Chemistry 2014

```
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9247571097 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
```

```
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860577320     A.U. after   12 cycles
             Convg  =    0.4202D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000088282    0.000043154   -0.000030057
      2        6           0.000032789    0.000015432    0.000040926
      3        6           0.000070032    0.000065276    0.000032073
      4        6           0.000042942   -0.000009299   -0.000069092
      5        6           0.000116871    0.000033548    0.000055759
      6        6           0.000033439   -0.000042015    0.000004688
      7        6          -0.000011040    0.000059700   -0.000056846
      8        6          -0.000150738   -0.000168411    0.000010525
      9        6           0.000091907   -0.000126101   -0.000048767
     10        6          -0.000028937   -0.000120166    0.000033379
     11        6           0.000024771    0.000042567    0.000034108
     12        1          -0.000091405   -0.000064118   -0.000007240
     13        6          -0.000043916    0.000055970   -0.000025318
     14        6           0.000030290   -0.000064804    0.000000604
     15        6           0.000143186    0.000133875    0.000046254
     16        1           0.000003739   -0.000009916    0.000039648
     17        1          -0.000120469    0.000042917    0.000029263
     18        1           0.000097873    0.000049432   -0.000016754
     19        1           0.000000135    0.000024607   -0.000019749
     20        1          -0.000044740   -0.000069113   -0.000027310
     21        1           0.000020879    0.000125628    0.000021641
     22        1           0.000091783    0.000002108   -0.000028536
     23        1           0.000138409   -0.000114652   -0.000039409
     24        6          -0.000107722   -0.000037237   -0.000061245
     25        1          -0.000028883    0.000007795   -0.000060305
     26        1          -0.000218128    0.000010346    0.000113816
     27        1          -0.000004782    0.000113476    0.000027944
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000218128 RMS     0.000071584
```

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000505269 RMS     0.000101315
 Search for a local minimum.
 Step number  24 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
21
                                                     20   23   22   24
 DE= -2.98D-06 DEPred=-2.43D-04 R= 1.23D-02
 Trust test= 1.23D-02 RLast= 5.01D-02 DXMaxT set to 5.00D-02
 Use linear search instead of GDIIS.
     Eigenvalues ---   -0.05603   0.00000   0.01219   0.01481
0.01752
     Eigenvalues ---    0.01795   0.01817   0.01830   0.01892
0.01976
     Eigenvalues ---    0.01976   0.02002   0.02012   0.02072
0.02105
     Eigenvalues ---    0.02119   0.02146   0.02209   0.02229
0.02250
     Eigenvalues ---    0.02277   0.02353   0.02445   0.06669
0.06915
     Eigenvalues ---    0.13662   0.15160   0.15800   0.15981
0.16000
     Eigenvalues ---    0.16000   0.16001   0.16003   0.16029
0.16161
     Eigenvalues ---    0.16217   0.20603   0.21992   0.22200
0.22611
     Eigenvalues ---    0.22965   0.23428   0.24443   0.24992
0.25387
     Eigenvalues ---    0.26601   0.28047   0.33476   0.33583
0.33626
     Eigenvalues ---    0.33632   0.33682   0.33682   0.33727
0.33934
     Eigenvalues ---    0.34115   0.34622   0.35651   0.36844
0.37180
     Eigenvalues ---    0.37350   0.38281   0.38927   0.39391
0.40376
     Eigenvalues ---    0.41125   0.42020   0.43388   0.45317
0.45908
     Eigenvalues ---    0.49321   0.49843   0.50890   0.51380
0.51961
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-5.60359467D-02 EMin=-5.60276614D-02
 RFO eigenvector is Hessian eigenvector with negative curvature.
 Taking step of  1.25D-01 in eigenvector direction.  Step.Grad= -
8.52D-05.
 Quartic linear search produced a step of  0.51790.
 Maximum step size (   0.050) exceeded in Quadratic search.
    -- Step size scaled by   0.400
 Iteration  1 RMS(Cart)=  0.01218131 RMS(Int)=  0.00012006
 Iteration  2 RMS(Cart)=  0.00013583 RMS(Int)=  0.00001193
 Iteration  3 RMS(Cart)=  0.00000002 RMS(Int)=  0.00001193
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58971   0.00016  -0.00013  -0.00110  -0.00122
2.58849
    R2        2.69211  -0.00012   0.00029   0.00389   0.00418
2.69629
    R3        2.05392   0.00002  -0.00006   0.00035   0.00029
2.05421
    R4        2.70475  -0.00002   0.00012   0.00073   0.00085
2.70560
    R5        2.05589   0.00001  -0.00007   0.00144   0.00137
2.05726
```

R6	2.73414	-0.00011	-0.00023	-0.00682	-0.00704
2.72710					
R7	2.64250	-0.00010	0.00022	0.00170	0.00192
2.64442					
R8	2.71206	-0.00006	0.00008	-0.00313	-0.00305
2.70900					
R9	2.67969	-0.00014	0.00011	-0.00683	-0.00671
2.67298					
R10	2.59499	0.00003	-0.00004	-0.00235	-0.00240
2.59260					
R11	2.04904	0.00002	0.00003	0.00371	0.00374
2.05278					
R12	2.05428	0.00005	-0.00013	0.00187	0.00174
2.05603					
R13	2.64179	-0.00010	0.00007	0.00060	0.00067
2.64246					
R14	2.05699	0.00001	-0.00008	0.00127	0.00119
2.05818					
R15	2.67837	0.00046	-0.00033	-0.00503	-0.00535
2.67302					
R16	2.86165	0.00027	-0.00004	-0.01559	-0.01563
2.84602					
R17	2.73723	0.00007	0.00012	-0.00172	-0.00161
2.73562					
R18	2.71296	0.00026	0.00010	0.00041	0.00051
2.71347					
R19	2.70542	0.00000	0.00022	0.00174	0.00196
2.70738					
R20	2.05587	0.00001	-0.00007	0.00145	0.00138
2.05724					
R21	2.58898	0.00006	-0.00020	-0.00259	-0.00280
2.58619					
R22	2.69246	-0.00018	0.00039	0.00390	0.00429
2.69675					
R23	2.05390	0.00002	-0.00007	0.00029	0.00022
2.05412					
R24	2.59424	0.00003	-0.00015	-0.00320	-0.00335
2.59089					
R25	2.05427	0.00005	-0.00014	0.00188	0.00175
2.05601					
R26	2.04877	-0.00017	0.00009	0.00192	0.00201
2.05077					
R27	2.07768	-0.00004	-0.00002	0.00188	0.00186
2.07955					
R28	2.06275	-0.00015	-0.00018	0.00042	0.00024
2.06298					
R29	2.06676	-0.00002	0.00030	0.00568	0.00598
2.07274					
A1	2.08978	-0.00002	0.00010	-0.00465	-0.00454
2.08524					
A2	2.10123	0.00014	-0.00015	0.00842	0.00827
2.10950					

This journal is © The Royal Society of Chemistry 2014

A3	2.09217	-0.00012	0.00004	-0.00378	-0.00374
2.08843					
A4	2.11602	0.00000	-0.00014	0.00011	-0.00003
2.11599					
A5	2.10339	0.00011	-0.00004	0.00699	0.00694
2.11033					
A6	2.06376	-0.00011	0.00018	-0.00709	-0.00691
2.05685					
A7	2.08484	-0.00002	0.00000	0.00297	0.00297
2.08780					
A8	2.11333	-0.00001	0.00013	-0.00037	-0.00024
2.11309					
A9	2.08501	0.00004	-0.00014	-0.00260	-0.00273
2.08228					
A10	2.04479	0.00004	0.00025	-0.00098	-0.00074
2.04405					
A11	2.09466	0.00011	0.00010	0.00562	0.00572
2.10038					
A12	2.14371	-0.00014	-0.00035	-0.00466	-0.00502
2.13869					
A13	2.12378	0.00002	-0.00024	0.00026	0.00002
2.12379					
A14	2.08689	-0.00003	-0.00019	0.00151	0.00133
2.08822					
A15	2.07241	0.00000	0.00042	-0.00176	-0.00133
2.07108					
A16	2.10702	-0.00002	0.00001	0.00227	0.00228
2.10930					
A17	2.08670	-0.00006	-0.00003	-0.00211	-0.00214
2.08456					
A18	2.08947	0.00008	0.00002	-0.00016	-0.00014
2.08932					
A19	2.11903	0.00002	-0.00007	-0.00186	-0.00193
2.11710					
A20	2.08227	-0.00001	0.00006	0.00123	0.00130
2.08357					
A21	2.08185	-0.00001	0.00000	0.00061	0.00061
2.08246					
A22	2.08798	-0.00009	0.00011	-0.00177	-0.00166
2.08631					
A23	2.08883	-0.00041	-0.00088	-0.01205	-0.01293
2.07590					
A24	2.10631	0.00051	0.00077	0.01378	0.01455
2.12085					
A25	2.09131	-0.00012	-0.00018	0.00067	0.00048
2.09180					
A26	2.14964	0.00031	0.00013	0.00497	0.00511
2.15475					
A27	2.04219	-0.00019	0.00005	-0.00565	-0.00560
2.03659					
A28	2.08746	0.00005	0.00012	-0.00001	0.00011
2.08757					

This journal is © The Royal Society of Chemistry 2014

A29	2.11026	-0.00010	-0.00014	-0.00425	-0.00439	2.10587
A30	2.08546	0.00006	0.00002	0.00425	0.00427	2.08973
A31	2.06300	-0.00014	0.00008	-0.00808	-0.00800	2.05501
A32	2.11672	0.00005	-0.00007	0.00123	0.00116	2.11788
A33	2.10345	0.00009	-0.00001	0.00686	0.00685	2.11030
A34	2.08885	-0.00001	0.00001	-0.00556	-0.00555	2.08330
A35	2.10176	0.00014	-0.00009	0.00888	0.00879	2.11055
A36	2.09257	-0.00012	0.00008	-0.00333	-0.00325	2.08932
A37	2.10774	0.00002	0.00009	0.00327	0.00336	2.11110
A38	2.08675	-0.00009	0.00000	-0.00231	-0.00231	2.08444
A39	2.08869	0.00007	-0.00009	-0.00096	-0.00105	2.08764
A40	2.12524	0.00008	-0.00011	0.00246	0.00235	2.12759
A41	2.08878	0.00003	-0.00007	0.00346	0.00339	2.09217
A42	2.06904	-0.00011	0.00017	-0.00589	-0.00572	2.06333
A43	1.95076	-0.00003	-0.00009	-0.00093	-0.00103	1.94973
A44	1.95672	0.00025	-0.00001	0.01868	0.01861	1.97533
A45	1.94499	0.00011	-0.00117	0.00856	0.00735	1.95234
A46	1.87534	-0.00012	0.00045	-0.00919	-0.00876	1.86658
A47	1.87317	-0.00009	0.00042	-0.00759	-0.00716	1.86601
A48	1.85779	-0.00015	0.00049	-0.01158	-0.01117	1.84662
D1	-0.00106	-0.00001	-0.00010	-0.00165	-0.00175	-0.00281
D2	3.13484	0.00001	-0.00025	0.00008	-0.00017	3.13467
D3	-3.13883	0.00000	0.00010	-0.00022	-0.00012	-3.13895
D4	-0.00293	0.00001	-0.00006	0.00152	0.00147	-0.00147
D5	0.00935	-0.00001	0.00037	0.00029	0.00066	0.01001
D6	-3.12962	-0.00001	0.00056	-0.00001	0.00055	-3.12907

This journal is © The Royal Society of Chemistry 2014

D7	-3.13604	-0.00001	0.00018	-0.00112	-0.00093	-3.13697
D8	0.00818	-0.00002	0.00037	-0.00141	-0.00104	0.00714
D9	-0.01266	0.00001	-0.00044	0.00024	-0.00020	-0.01286
D10	3.12583	0.00001	-0.00060	-0.00057	-0.00118	3.12465
D11	3.13450	0.00000	-0.00029	-0.00149	-0.00178	3.13272
D12	-0.01019	-0.00001	-0.00045	-0.00231	-0.00276	-0.01295
D13	0.01774	0.00000	0.00071	0.00239	0.00310	0.02084
D14	-3.13171	-0.00002	0.00005	-0.00169	-0.00166	-3.13337
D15	-3.12080	0.00001	0.00086	0.00320	0.00406	-3.11674
D16	0.01293	-0.00001	0.00021	-0.00089	-0.00070	0.01223
D17	-3.12223	0.00000	0.00092	0.00094	0.00186	-3.12037
D18	0.00976	-0.00001	0.00082	-0.00103	-0.00021	0.00955
D19	0.01626	0.00000	0.00076	0.00013	0.00089	0.01716
D20	-3.13493	-0.00002	0.00066	-0.00184	-0.00117	-3.13611
D21	-0.00992	-0.00002	-0.00045	-0.00377	-0.00422	-0.01413
D22	3.11627	0.00001	-0.00076	-0.00248	-0.00324	3.11304
D23	3.13978	0.00000	0.00022	0.00039	0.00060	3.14038
D24	-0.01722	0.00003	-0.00008	0.00168	0.00158	-0.01564
D25	-0.04256	0.00004	-0.00131	0.00142	0.00012	-0.04244
D26	3.11188	0.00006	-0.00146	0.00517	0.00369	3.11557
D27	3.09071	0.00002	-0.00200	-0.00288	-0.00488	3.08583
D28	-0.03804	0.00004	-0.00215	0.00087	-0.00131	-0.03935
D29	-0.00357	0.00002	-0.00008	0.00249	0.00241	-0.00116
D30	3.13540	0.00002	-0.00027	0.00279	0.00252	3.13791
D31	-3.12988	0.00000	0.00023	0.00119	0.00141	-3.12847
D32	0.00909	0.00000	0.00004	0.00148	0.00152	0.01060

D33	-0.01531	0.00001	-0.00061	0.00011	-0.00049	-0.01580
D34	3.12237	0.00001	-0.00073	-0.00029	-0.00102	3.12135
D35	3.13589	0.00002	-0.00051	0.00208	0.00157	3.13746
D36	-0.00962	0.00002	-0.00063	0.00167	0.00105	-0.00857
D37	0.04345	-0.00004	0.00145	-0.00127	0.00019	0.04364
D38	-3.08860	-0.00003	0.00149	-0.00030	0.00120	-3.08740
D39	-3.11111	-0.00007	0.00159	-0.00525	-0.00369	-3.11480
D40	0.04002	-0.00006	0.00163	-0.00429	-0.00267	0.03735
D41	1.44898	-0.00006	-0.01049	-0.00534	-0.01584	1.43314
D42	-2.72732	-0.00006	-0.00999	-0.00467	-0.01469	-2.74201
D43	-0.64694	0.00000	-0.01017	-0.00091	-0.01105	-0.65799
D44	-1.67963	-0.00002	-0.01064	-0.00143	-0.01207	-1.69170
D45	0.42725	-0.00003	-0.01013	-0.00076	-0.01092	0.41634
D46	2.50763	0.00003	-0.01031	0.00300	-0.00728	2.50035
D47	-0.01486	0.00002	-0.00051	0.00043	-0.00009	-0.01495
D48	3.13059	0.00002	-0.00039	0.00085	0.00045	3.13104
D49	3.11776	0.00001	-0.00055	-0.00042	-0.00098	3.11679
D50	-0.01997	0.00001	-0.00043	0.00000	-0.00044	-0.02041
D51	-3.13909	0.00000	0.00016	0.00073	0.00089	-3.13820
D52	0.01916	-0.00003	0.00039	-0.00124	-0.00086	0.01830
D53	0.01179	0.00001	0.00020	0.00164	0.00184	0.01364
D54	-3.11314	-0.00002	0.00043	-0.00033	0.00009	-3.11305
D55	0.01182	0.00000	0.00032	0.00102	0.00133	0.01315
D56	-3.12385	-0.00002	0.00043	-0.00088	-0.00044	-3.12429
D57	-3.13368	0.00000	0.00020	0.00061	0.00080	-3.13289
D58	0.01383	-0.00002	0.00032	-0.00129	-0.00098	0.01285

```
   D59        0.00145   0.00001   0.00004   0.00105   0.00109
0.00254
   D60        3.13849   0.00001   0.00001   0.00064   0.00065
3.13914
   D61       -3.13408  -0.00001   0.00016  -0.00084  -0.00069  -
3.13477
   D62        0.00296  -0.00001   0.00013  -0.00125  -0.00113
0.00183
   D63       -0.01016   0.00001  -0.00028   0.00062   0.00034  -
0.00982
   D64        3.12831   0.00002  -0.00046   0.00116   0.00070
3.12901
   D65        3.13596   0.00001  -0.00025   0.00100   0.00074
3.13670
   D66       -0.00875   0.00002  -0.00043   0.00153   0.00110  -
0.00765
   D67        0.00318  -0.00002   0.00015  -0.00201  -0.00186
0.00132
   D68        3.12829   0.00001  -0.00007   0.00003  -0.00005
3.12824
   D69       -3.13529  -0.00002   0.00033  -0.00254  -0.00221  -
3.13751
   D70       -0.01018   0.00000   0.00010  -0.00050  -0.00041  -
0.01059
         Item               Value     Threshold  Converged?
 Maximum Force            0.000505     0.000450     NO
 RMS     Force            0.000101     0.000300     YES
 Maximum Displacement     0.068368     0.001800     NO
 RMS     Displacement     0.012205     0.001200     NO
 Predicted change in Energy=-1.044692D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.791639   -5.423551    0.013143
      2          6           0       -3.422560   -5.392842   -0.017652
      3          6           0       -2.707862   -4.152329   -0.032528
      4          6           0       -3.438725   -2.907973   -0.030989
      5          6           0       -4.869236   -2.990479    0.012318
      6          6           0       -5.521085   -4.197474    0.034256
      7          6           0       -1.308807   -4.124948   -0.043695
      8          6           0       -2.748257   -1.673708   -0.055595
      9          6           0       -1.334020   -1.665191   -0.029563
     10          6           0       -0.605733   -2.916276   -0.032884
     11          6           0        0.826841   -2.904543   -0.019598
     12          1           0        1.341615   -3.863725   -0.030936
     13          6           0        1.528905   -1.730199    0.011303
```

14	6	0	0.820332	-0.491688	0.033866
15	6	0	-0.550254	-0.462825	0.013470
16	1	0	-0.756048	-5.063378	-0.050074
17	1	0	-5.328088	-6.368907	0.026763
18	1	0	-2.842557	-6.314071	-0.027773
19	1	0	-5.459372	-2.078958	0.042024
20	1	0	-6.608191	-4.222616	0.070576
21	1	0	2.615830	-1.729301	0.023499
22	1	0	1.377257	0.442248	0.070358
23	1	0	-1.043700	0.503219	0.044756
24	6	0	-3.542786	-0.394691	-0.087519
25	1	0	-3.881037	-0.100387	0.917448
26	1	0	-2.982425	0.449193	-0.494494
27	1	0	-4.439828	-0.486614	-0.711966

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.369769	0.000000			
3	C	2.441356	1.431743	0.000000		
4	C	2.856652	2.484958	1.443117	0.000000	
5	C	2.434310	2.804482	2.454270	1.433542	0.000000
6	C	1.426816	2.415659	2.814377	2.450162	1.371942
7	C	3.717488	2.464992	1.399367	2.453108	3.737219
8	C	4.271002	3.779958	2.479057	1.414482	2.497408
9	C	5.107075	4.272882	2.841356	2.444236	3.775697
10	C	4.879586	3.750750	2.438601	2.833005	4.264388
11	C	6.157417	4.924332	3.748501	4.265582	5.696814
12	H	6.328649	5.003573	4.059748	4.874947	6.272088
13	C	7.320528	6.158961	4.880454	5.105515	6.521082
14	C	7.471139	6.482753	5.084570	4.897162	6.214145
15	C	6.526726	5.705803	4.274322	3.784705	5.004262
16	H	4.052125	2.686984	2.154042	3.441350	4.606421
17	H	1.087043	2.141428	3.432539	3.943488	3.409477
18	H	2.143273	1.088655	2.165939	3.457880	3.892981
19	H	3.410719	3.890243	3.446046	2.185317	1.086284
20	H	2.178395	3.394916	3.902324	3.432800	2.132023
21	H	8.277571	7.062958	5.849436	6.168458	7.590580
22	H	8.512706	7.556075	6.148896	5.867532	7.127809
23	H	7.012464	6.358177	4.944647	4.168706	5.180898
24	C	5.182586	5.000085	3.849670	2.516070	2.916770
25	H	5.475677	5.393950	4.324006	2.996283	3.185659
26	H	6.166042	5.877965	4.632796	3.419592	3.955787
27	H	5.002290	5.058456	4.110816	2.707197	2.641650

		6	7	8	9	10
6	C	0.000000				
7	C	4.213623	0.000000			
8	C	3.750472	2.842663	0.000000		
9	C	4.893673	2.459927	1.414501	0.000000	
10	C	5.080026	1.398327	2.476873	1.447628	0.000000
11	C	6.478482	2.459870	3.781213	2.491067	1.432684
12	H	6.871120	2.663295	4.639378	3.463030	2.165601

This journal is © The Royal Society of Chemistry 2014

13	C	7.469292	3.713551	4.278058	2.863955	2.442419
14	C	7.344822	4.211867	3.760319	2.454051	2.813670
15	C	6.217491	3.740296	2.510423	1.435906	2.454516
16	H	4.843808	1.089144	3.931766	3.447049	2.152426
17	H	2.180007	4.603796	5.357911	6.170956	5.850202
18	H	3.414432	2.672994	4.641404	4.887511	4.067975
19	H	2.119428	4.628241	2.742974	4.146668	4.925904
20	H	1.088003	5.301515	4.627304	5.862365	6.143836
21	H	8.503022	4.598524	5.364958	3.950727	3.433738
22	H	8.313570	5.299739	4.638211	3.435449	3.901614
23	H	6.491810	4.636598	2.766694	2.189021	3.448302
24	C	4.288316	4.348263	1.506048	2.548759	3.871389
25	H	4.500656	4.872089	2.169180	3.135719	4.422666
26	H	5.321267	4.891521	2.180407	2.721033	4.145857
27	H	3.936552	4.846375	2.168278	3.391277	4.589629

		11	12	13	14	15
11	C	0.000000				
12	H	1.088645	0.000000			
13	C	1.368552	2.142147	0.000000		
14	C	2.413456	3.412706	1.427057	0.000000	
15	C	2.803475	3.891948	2.434983	1.371041	0.000000
16	H	2.677131	2.416552	4.041641	4.836565	4.605592
17	H	7.063082	7.124901	8.278660	8.505576	7.596690
18	H	5.008934	4.848865	6.334279	6.879003	6.284380
19	H	6.340494	7.031653	6.997042	6.477204	5.168380
20	H	7.551499	7.958550	8.510463	8.312888	7.130070
21	H	2.140919	2.486434	1.086994	2.180735	3.410007
22	H	3.392943	4.307312	2.178534	1.087996	2.130186
23	H	3.887918	4.976510	3.406988	2.112953	1.085223
24	C	5.039604	5.991223	5.245511	4.365883	2.995011
25	H	5.559268	6.506783	5.722312	4.799656	3.470253
26	H	5.097409	6.124824	5.035641	3.952895	2.646746
27	H	5.836400	6.730064	6.139658	5.312775	3.956718

		16	17	18	19	20
16	H	0.000000				
17	H	4.755404	0.000000			
18	H	2.432745	2.486735	0.000000		
19	H	5.571041	4.291985	4.978833	0.000000	
20	H	5.913460	2.499430	4.308579	2.432255	0.000000
21	H	4.742472	9.199554	7.128585	8.082790	9.555176
22	H	5.905710	9.558002	7.966449	7.286754	9.248153
23	H	5.574831	8.098298	7.050999	5.115253	7.300530
24	C	5.437273	6.236315	5.960952	2.554768	4.906598
25	H	5.944151	6.494738	6.370381	2.678107	5.014712
26	H	5.961770	7.229131	6.780791	3.579758	5.940646
27	H	5.912284	5.994673	6.081007	2.035566	4.389975

		21	22	23	24	25
21	H	0.000000				
22	H	2.500377	0.000000			
23	H	4.286812	2.421860	0.000000		
24	C	6.302543	4.993217	2.658791	0.000000	
25	H	6.757350	5.353659	3.029259	1.100448	0.000000

This journal is © The Royal Society of Chemistry 2014

```
   26  H    6.029479   4.396128   2.013049   1.091684   1.761567
   27  H    7.201909   5.942499   3.617470   1.096845   1.765335
                  26         27
   26  H    0.000000
   27  H    1.745581   0.000000
 Stoichiometry    C15H12
 Framework group  C1[X(C15H12)]
 Deg. of freedom    75
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.653587   -1.004256    0.023181
      2          6           0       -2.454431   -1.665433   -0.010569
      3          6           0       -1.213213   -0.951898   -0.022129
      4          6           0       -1.219917    0.491180   -0.014009
      5          6           0       -2.498213    1.138381    0.032187
      6          6           0       -3.668251    0.422217    0.050800
      7          6           0        0.010187   -1.631103   -0.036332
      8          6           0       -0.002788    1.211531   -0.035267
      9          6           0        1.224259    0.508219   -0.012381
     10          6           0        1.225356   -0.939375   -0.022305
     11          6           0        2.469873   -1.649062   -0.012193
     12          1           0        2.433027   -2.736961   -0.028494
     13          6           0        3.666920   -0.986598    0.021790
     14          6           0        3.676549    0.440131    0.050861
     15          6           0        2.506025    1.153805    0.033661
     16          1           0        0.016609   -2.720168   -0.047678
     17          1           0       -4.592391   -1.552149    0.034256
     18          1           0       -2.415810   -2.753298   -0.025650
     19          1           0       -2.550474    2.222854    0.066837
     20          1           0       -4.620812    0.946510    0.089463
     21          1           0        4.607141   -1.531982    0.031546
     22          1           0        4.627317    0.967634    0.089807
     23          1           0        2.564759    2.236832    0.069890
     24          6           0       -0.047122    2.716717   -0.060329
     25          1           0       -0.191760    3.136538    0.946555
     26          1           0        0.861392    3.166657   -0.465210
     27          1           0       -0.868872    3.090791   -0.683118
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3963656      0.4485640
0.3403338
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
```

```
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       879.5423382111 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
```

```
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860358494     A.U. after   12 cycles
             Convg  =    0.4070D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.001221067    0.001842638    0.000069379
      2        6           0.001368326   -0.000419700   -0.000155067
      3        6           0.002008277   -0.001432656   -0.000007665
      4        6          -0.001920447   -0.001300501    0.000402871
      5        6          -0.001921562    0.001068211   -0.000093580
      6        6          -0.000900401   -0.002159986    0.000052536
      7        6          -0.000409499    0.000078714   -0.000001631
      8        6           0.000676671   -0.001478627   -0.000528779
      9        6           0.002632412    0.000857765   -0.000011926
     10        6           0.000058047   -0.001600588    0.000040420
     11        6          -0.000628511   -0.001600153   -0.000138909
     12        1           0.000327049    0.000683271    0.000057837
     13        6          -0.000935842    0.002262466    0.000043108
     14        6           0.002574522   -0.000345683    0.000046276
     15        6          -0.001660856    0.001676413   -0.000175004
     16        1          -0.000247992    0.000359368   -0.000011834
     17        1           0.000509523   -0.000092214   -0.000022350
     18        1          -0.000777956    0.000042690    0.000054249
     19        1           0.000734169   -0.001527569   -0.000023798
     20        1           0.000537030   -0.000039038    0.000026511
     21        1          -0.000156261   -0.000467822   -0.000005834
     22        1          -0.000244448   -0.000483750    0.000007457
     23        1          -0.000507747   -0.000791032   -0.000193113
     24        6          -0.003554136    0.006108192   -0.000253382
     25        1           0.000033859   -0.000243345   -0.000251801
     26        1           0.001699733   -0.000588974    0.000137581
     27        1           0.001927106   -0.000408093    0.000936447
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.006108192 RMS     0.001256946


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.005015628 RMS     0.001004327
```

```
 Search for a local minimum.
 Step number  25 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
21
                                                     20   23   22   25
24
 DE=  2.19D-04 DEPred=-1.04D-04 R=-2.09D+00
 Trust test=-2.09D+00 RLast= 5.78D-02 DXMaxT set to 5.00D-02
 Use linear search instead of GDIIS.
 Quartic linear search produced a step of -0.93953.
 Iteration  1 RMS(Cart)=  0.01147836 RMS(Int)=  0.00010555
 Iteration  2 RMS(Cart)=  0.00011863 RMS(Int)=  0.00000068
 Iteration  3 RMS(Cart)=  0.00000001 RMS(Int)=  0.00000068
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.58849   0.00033   0.00115   0.00000   0.00115
2.58963
    R2        2.69629  -0.00139  -0.00393   0.00000  -0.00393
2.69236
    R3        2.05421  -0.00017  -0.00027   0.00000  -0.00027
2.05394
    R4        2.70560  -0.00010  -0.00080   0.00000  -0.00080
2.70480
    R5        2.05726  -0.00045  -0.00129   0.00000  -0.00129
2.05597
    R6        2.72710   0.00237   0.00662   0.00000   0.00662
2.73371
    R7        2.64442  -0.00036  -0.00180   0.00000  -0.00180
2.64262
    R8        2.70900   0.00198   0.00287   0.00000   0.00287
2.71187
    R9        2.67298   0.00462   0.00630   0.00000   0.00630
2.67929
   R10        2.59260   0.00105   0.00225   0.00000   0.00225
2.59485
   R11        2.05278  -0.00168  -0.00352   0.00000  -0.00352
2.04926
   R12        2.05603  -0.00054  -0.00164   0.00000  -0.00164
2.05439
   R13        2.64246  -0.00038  -0.00063   0.00000  -0.00063
2.64183
   R14        2.05818  -0.00044  -0.00112   0.00000  -0.00112
2.05706
```

This journal is © The Royal Society of Chemistry 2014

R15	2.67302	0.00115	0.00503	0.00000	0.00503
2.67805					
R16	2.84602	0.00407	0.01468	0.00000	0.01468
2.86070					
R17	2.73562	0.00031	0.00151	0.00000	0.00151
2.73713					
R18	2.71347	-0.00005	-0.00048	0.00000	-0.00048
2.71299					
R19	2.70738	-0.00025	-0.00184	0.00000	-0.00184
2.70554					
R20	2.05724	-0.00045	-0.00129	0.00000	-0.00129
2.05595					
R21	2.58619	0.00111	0.00263	0.00000	0.00263
2.58881					
R22	2.69675	-0.00103	-0.00403	0.00000	-0.00403
2.69272					
R23	2.05412	-0.00016	-0.00021	0.00000	-0.00021
2.05391					
R24	2.59089	0.00119	0.00315	0.00000	0.00315
2.59404					
R25	2.05601	-0.00054	-0.00164	0.00000	-0.00164
2.05437					
R26	2.05077	-0.00048	-0.00188	0.00000	-0.00188
2.04889					
R27	2.07955	-0.00030	-0.00175	0.00000	-0.00175
2.07780					
R28	2.06298	0.00036	-0.00022	0.00000	-0.00022
2.06276					
R29	2.07274	-0.00208	-0.00562	0.00000	-0.00562
2.06712					
A1	2.08524	0.00090	0.00427	0.00000	0.00427
2.08951					
A2	2.10950	-0.00096	-0.00777	0.00000	-0.00777
2.10173					
A3	2.08843	0.00005	0.00351	0.00000	0.00351
2.09194					
A4	2.11599	0.00020	0.00003	0.00000	0.00003
2.11602					
A5	2.11033	-0.00075	-0.00652	0.00000	-0.00652
2.10381					
A6	2.05685	0.00056	0.00649	0.00000	0.00649
2.06334					
A7	2.08780	-0.00027	-0.00279	0.00000	-0.00279
2.08502					
A8	2.11309	-0.00055	0.00022	0.00000	0.00022
2.11332					
A9	2.08228	0.00083	0.00257	0.00000	0.00257
2.08485					
A10	2.04405	-0.00071	0.00070	0.00000	0.00070
2.04474					
A11	2.10038	-0.00182	-0.00537	0.00000	-0.00537
2.09500					

This journal is © The Royal Society of Chemistry 2014

A12	2.13869	0.00252	0.00472	0.00000	0.00472
2.14341					
A13	2.12379	0.00007	-0.00002	0.00000	-0.00002
2.12378					
A14	2.08822	0.00018	-0.00125	0.00000	-0.00125
2.08697					
A15	2.07108	-0.00026	0.00125	0.00000	0.00125
2.07233					
A16	2.10930	-0.00019	-0.00214	0.00000	-0.00214
2.10716					
A17	2.08456	0.00004	0.00201	0.00000	0.00201
2.08657					
A18	2.08932	0.00015	0.00013	0.00000	0.00013
2.08946					
A19	2.11710	0.00061	0.00181	0.00000	0.00181
2.11892					
A20	2.08357	-0.00034	-0.00122	0.00000	-0.00122
2.08234					
A21	2.08246	-0.00027	-0.00058	0.00000	-0.00058
2.08188					
A22	2.08631	-0.00029	0.00156	0.00000	0.00156
2.08788					
A23	2.07590	0.00502	0.01215	0.00000	0.01215
2.08805					
A24	2.12085	-0.00473	-0.01367	0.00000	-0.01367
2.10719					
A25	2.09180	0.00047	-0.00046	0.00000	-0.00046
2.09134					
A26	2.15475	-0.00179	-0.00480	0.00000	-0.00480
2.14995					
A27	2.03659	0.00132	0.00526	0.00000	0.00526
2.04185					
A28	2.08757	0.00020	-0.00010	0.00000	-0.00010
2.08747					
A29	2.10587	0.00080	0.00412	0.00000	0.00412
2.10999					
A30	2.08973	-0.00099	-0.00401	0.00000	-0.00401
2.08571					
A31	2.05501	0.00070	0.00751	0.00000	0.00751
2.06252					
A32	2.11788	-0.00013	-0.00109	0.00000	-0.00109
2.11679					
A33	2.11030	-0.00056	-0.00643	0.00000	-0.00643
2.10386					
A34	2.08330	0.00102	0.00521	0.00000	0.00521
2.08851					
A35	2.11055	-0.00099	-0.00826	0.00000	-0.00826
2.10229					
A36	2.08932	-0.00003	0.00305	0.00000	0.00305
2.09237					
A37	2.11110	-0.00064	-0.00316	0.00000	-0.00316
2.10794					

This journal is © The Royal Society of Chemistry 2014

A38	2.08444	0.00028	0.00217	0.00000	0.00217	2.08661
A39	2.08764	0.00036	0.00099	0.00000	0.00099	2.08863
A40	2.12759	-0.00057	-0.00221	0.00000	-0.00221	2.12539
A41	2.09217	-0.00055	-0.00318	0.00000	-0.00318	2.08899
A42	2.06333	0.00112	0.00537	0.00000	0.00537	2.06870
A43	1.94973	0.00042	0.00097	0.00000	0.00097	1.95070
A44	1.97533	-0.00230	-0.01749	0.00000	-0.01748	1.95785
A45	1.95234	-0.00041	-0.00691	0.00000	-0.00691	1.94543
A46	1.86658	0.00079	0.00823	0.00000	0.00823	1.87481
A47	1.86601	0.00040	0.00673	0.00000	0.00673	1.87274
A48	1.84662	0.00133	0.01049	0.00000	0.01050	1.85712
D1	-0.00281	0.00002	0.00164	0.00000	0.00164	-0.00116
D2	3.13467	-0.00002	0.00016	0.00000	0.00016	3.13483
D3	-3.13895	0.00002	0.00011	0.00000	0.00011	-3.13884
D4	-0.00147	-0.00002	-0.00138	0.00000	-0.00138	-0.00284
D5	0.01001	0.00001	-0.00062	0.00000	-0.00062	0.00939
D6	-3.12907	0.00002	-0.00052	0.00000	-0.00052	-3.12958
D7	-3.13697	0.00001	0.00087	0.00000	0.00087	-3.13610
D8	0.00714	0.00002	0.00098	0.00000	0.00098	0.00811
D9	-0.01286	-0.00003	0.00019	0.00000	0.00019	-0.01267
D10	3.12465	-0.00004	0.00111	0.00000	0.00111	3.12576
D11	3.13272	0.00001	0.00167	0.00000	0.00167	3.13439
D12	-0.01295	0.00001	0.00259	0.00000	0.00259	-0.01036
D13	0.02084	0.00000	-0.00291	0.00000	-0.00291	0.01793
D14	-3.13337	0.00002	0.00156	0.00000	0.00156	-3.13181
D15	-3.11674	0.00001	-0.00381	0.00000	-0.00381	-3.12056

This journal is © The Royal Society of Chemistry 2014

D16	0.01223	0.00003	0.00065	0.00000	0.00066	0.01289
D17	-3.12037	-0.00005	-0.00175	0.00000	-0.00175	-3.12212
D18	0.00955	0.00000	0.00019	0.00000	0.00019	0.00975
D19	0.01716	-0.00006	-0.00084	0.00000	-0.00084	0.01632
D20	-3.13611	-0.00001	0.00110	0.00000	0.00110	-3.13501
D21	-0.01413	0.00003	0.00396	0.00000	0.00396	-0.01017
D22	3.11304	-0.00001	0.00304	0.00000	0.00304	3.11608
D23	3.14038	0.00004	-0.00056	0.00000	-0.00056	3.13982
D24	-0.01564	-0.00001	-0.00149	0.00000	-0.00149	-0.01712
D25	-0.04244	0.00006	-0.00011	0.00000	-0.00011	-0.04255
D26	3.11557	0.00008	-0.00347	0.00000	-0.00346	3.11210
D27	3.08583	0.00006	0.00459	0.00000	0.00459	3.09042
D28	-0.03935	0.00008	0.00123	0.00000	0.00123	-0.03812
D29	-0.00116	-0.00003	-0.00226	0.00000	-0.00226	-0.00342
D30	3.13791	-0.00004	-0.00236	0.00000	-0.00236	3.13555
D31	-3.12847	0.00001	-0.00133	0.00000	-0.00133	-3.12979
D32	0.01060	0.00000	-0.00143	0.00000	-0.00143	0.00918
D33	-0.01580	0.00000	0.00046	0.00000	0.00046	-0.01534
D34	3.12135	0.00004	0.00095	0.00000	0.00095	3.12231
D35	3.13746	-0.00005	-0.00148	0.00000	-0.00148	3.13598
D36	-0.00857	0.00000	-0.00098	0.00000	-0.00098	-0.00956
D37	0.04364	-0.00007	-0.00018	0.00000	-0.00018	0.04346
D38	-3.08740	-0.00019	-0.00113	0.00000	-0.00113	-3.08852
D39	-3.11480	0.00000	0.00346	0.00000	0.00346	-3.11134
D40	0.03735	-0.00012	0.00251	0.00000	0.00251	0.03986
D41	1.43314	0.00003	0.01488	0.00000	0.01488	1.44802

This journal is © The Royal Society of Chemistry 2014

D42	-2.74201	-0.00030	0.01380	0.00000	0.01380	-2.72820
D43	-0.65799	-0.00048	0.01038	0.00000	0.01038	-0.64761
D44	-1.69170	0.00001	0.01134	0.00000	0.01134	-1.68036
D45	0.41634	-0.00032	0.01026	0.00000	0.01026	0.42660
D46	2.50035	-0.00050	0.00684	0.00000	0.00683	2.50719
D47	-0.01495	0.00005	0.00008	0.00000	0.00008	-0.01487
D48	3.13104	0.00000	-0.00042	0.00000	-0.00042	3.13062
D49	3.11679	0.00014	0.00092	0.00000	0.00092	3.11771
D50	-0.02041	0.00009	0.00041	0.00000	0.00041	-0.01999
D51	-3.13820	0.00000	-0.00084	0.00000	-0.00084	-3.13904
D52	0.01830	-0.00002	0.00081	0.00000	0.00081	0.01911
D53	0.01364	-0.00011	-0.00173	0.00000	-0.00173	0.01190
D54	-3.11305	-0.00013	-0.00008	0.00000	-0.00008	-3.11313
D55	0.01315	-0.00008	-0.00125	0.00000	-0.00125	0.01190
D56	-3.12429	-0.00007	0.00041	0.00000	0.00041	-3.12388
D57	-3.13289	-0.00003	-0.00075	0.00000	-0.00075	-3.13364
D58	0.01285	-0.00002	0.00092	0.00000	0.00092	0.01377
D59	0.00254	-0.00005	-0.00102	0.00000	-0.00102	0.00152
D60	3.13914	-0.00001	-0.00061	0.00000	-0.00061	3.13853
D61	-3.13477	-0.00004	0.00065	0.00000	0.00065	-3.13412
D62	0.00183	0.00000	0.00106	0.00000	0.00106	0.00289
D63	-0.00982	0.00003	-0.00032	0.00000	-0.00032	-0.01014
D64	3.12901	0.00004	-0.00066	0.00000	-0.00066	3.12835
D65	3.13670	-0.00001	-0.00069	0.00000	-0.00069	3.13600
D66	-0.00765	0.00001	-0.00103	0.00000	-0.00103	-0.00869
D67	0.00132	0.00006	0.00174	0.00000	0.00174	0.00307

```
   D68        3.12824   0.00007   0.00005   0.00000   0.00005
3.12829
   D69       -3.13751   0.00004   0.00208   0.00000   0.00208  -
3.13543
   D70       -0.01059   0.00005   0.00038   0.00000   0.00038  -
0.01020
         Item               Value     Threshold  Converged?
 Maximum Force            0.005016     0.000450     NO
 RMS     Force            0.001004     0.000300     NO
 Maximum Displacement     0.064261     0.001800     NO
 RMS     Displacement     0.011468     0.001200     NO
 Predicted change in Energy=-9.622365D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792527   -5.427879    0.012396
      2          6           0       -3.422853   -5.396297   -0.018025
      3          6           0       -2.709064   -4.155726   -0.030725
      4          6           0       -3.445877   -2.910816   -0.027072
      5          6           0       -4.877787   -2.997335    0.012301
      6          6           0       -5.526902   -4.207172    0.033337
      7          6           0       -1.310994   -4.127250   -0.042825
      8          6           0       -2.751315   -1.675020   -0.051540
      9          6           0       -1.334385   -1.667151   -0.027111
     10          6           0       -0.606845   -2.919588   -0.032028
     11          6           0        0.824730   -2.903428   -0.020908
     12          1           0        1.349303   -3.856501   -0.032504
     13          6           0        1.522615   -1.724992    0.010450
     14          6           0        0.816403   -0.487616    0.034439
     15          6           0       -0.555914   -0.461602    0.014549
     16          1           0       -0.758957   -5.065397   -0.051802
     17          1           0       -5.320983   -6.377586    0.024299
     18          1           0       -2.848650   -6.320351   -0.027948
     19          1           0       -5.468346   -2.088258    0.040445
     20          1           0       -6.613092   -4.235432    0.068810
     21          1           0        2.609437   -1.728536    0.021409
     22          1           0        1.371839    0.446160    0.071823
     23          1           0       -1.056106    0.499817    0.046595
     24          6           0       -3.531661   -0.378294   -0.086288
     25          1           0       -3.855086   -0.070010    0.918353
     26          1           0       -2.948420    0.442391   -0.507981
     27          1           0       -4.429996   -0.468144   -0.703929
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
```

This journal is © The Royal Society of Chemistry 2014

2	C	1.370376	0.000000			
3	C	2.441526	1.431318	0.000000		
4	C	2.854930	2.485603	1.446619	0.000000	
5	C	2.432039	2.805845	2.459080	1.435061	0.000000
6	C	1.424736	2.417370	2.819035	2.452519	1.373134
7	C	3.716955	2.463948	1.398413	2.457171	3.741892
8	C	4.272539	3.781533	2.481153	1.417819	2.504890
9	C	5.109147	4.274144	2.843020	2.450531	3.785054
10	C	4.879901	3.750225	2.438722	2.839051	4.271879
11	C	6.158534	4.925075	3.749140	4.270618	5.703386
12	H	6.339820	5.014445	4.069384	4.887546	6.286241
13	C	7.320683	6.159298	4.880295	5.108181	6.525642
14	C	7.474408	6.486077	5.088044	4.903338	6.222779
15	C	6.527848	5.707155	4.276057	3.788440	5.010842
16	H	4.050333	2.684581	2.151944	3.444179	4.609311
17	H	1.086899	2.137198	3.429549	3.941719	3.409202
18	H	2.139344	1.087973	2.169123	3.461446	3.893771
19	H	3.407432	3.889805	3.448641	2.184386	1.084424
20	H	2.177055	3.395993	3.906109	3.434392	2.132454
21	H	8.274919	7.059925	5.846403	6.169844	7.593975
22	H	8.515120	7.558534	6.151556	5.872773	7.135757
23	H	7.007110	6.353725	4.940883	4.165195	5.180395
24	C	5.205558	5.019647	3.866361	2.534667	2.946380
25	H	5.514192	5.425215	4.348240	3.021831	3.230492
26	H	6.175079	5.878386	4.629011	3.423848	3.978048
27	H	5.024293	5.076563	4.124690	2.719057	2.666516

		6	7	8	9	10
6	C	0.000000				
7	C	4.217353	0.000000			
8	C	3.758042	2.843947	0.000000		
9	C	4.902301	2.460261	1.417162	0.000000	
10	C	5.086168	1.397995	2.479533	1.448426	0.000000
11	C	6.484282	2.461613	3.781273	2.488011	1.431709
12	H	6.885456	2.674059	4.644813	3.463447	2.168945
13	C	7.473783	3.715243	4.274672	2.857833	2.442021
14	C	7.353408	4.216482	3.761108	2.453769	2.818606
15	C	6.224176	3.743049	2.509290	1.435654	2.458955
16	H	4.845317	1.088552	3.932448	3.446710	2.151285
17	H	2.180179	4.598753	5.359391	6.171208	5.846710
18	H	3.412084	2.678488	4.646411	4.893391	4.073193
19	H	2.119735	4.631199	2.749815	4.155903	4.932602
20	H	1.087137	5.304376	4.635031	5.871117	6.149522
21	H	8.505515	4.596492	5.361515	3.944598	3.430150
22	H	8.321514	5.303472	4.638429	3.435043	3.905667
23	H	6.491835	4.634945	2.759217	2.186005	3.449688
24	C	4.319213	4.357514	1.513818	2.548072	3.875006
25	H	4.549102	4.884411	2.176019	3.130287	4.424296
26	H	5.344158	4.876388	2.174998	2.699353	4.124610
27	H	3.965740	4.853276	2.167978	3.387994	4.591025

		11	12	13	14	15
11	C	0.000000				
12	H	1.087961	0.000000			

This journal is © The Royal Society of Chemistry 2014

```
   13  C    1.369941   2.138975   0.000000
   14  C    2.416460   3.411429   1.424924   0.000000
   15  C    2.805343   3.893251   2.432376   1.372708   0.000000
   16  H    2.680136   2.430343   4.045709   4.842032   4.608748
   17  H    7.059859   7.131046   8.275365   8.506430   7.596370
   18  H    5.016885   4.867586   6.342457   6.888926   6.291533
   19  H    6.345949   7.043603   7.000457   6.485381   5.174811
   20  H    7.556684   7.972050   8.514426   8.321340   7.136816
   21  H    2.137134   2.473677   1.086883   2.180601   3.409489
   22  H    3.395241   4.303984   2.177245   1.087127   2.131559
   23  H    3.888981   4.976922   3.406007   2.116947   1.084226
   24  C    5.035744   5.993715   5.231506   4.351113   2.978620
   25  H    5.550779   6.505944   5.699380   4.772684   3.443072
   26  H    5.066399   6.097292   4.995645   3.915741   2.610426
   27  H    5.831746   6.732909   6.125649   5.298138   3.940148
                 16         17         18         19         20
   16  H    0.000000
   17  H    4.747600   0.000000
   18  H    2.437682   2.473547   0.000000
   19  H    5.572272   4.291889   4.977761   0.000000
   20  H    5.913906   2.502069   4.304332   2.433435   0.000000
   21  H    4.741949   9.192673   7.132876   8.085811   9.557291
   22  H    5.910401   9.558223   7.975472   7.294683   9.256157
   23  H    5.574010   8.092486   7.052196   5.115274   7.300902
   24  C    5.445917   6.261422   5.981468   2.586656   4.939311
   25  H    5.956602   6.537102   6.401185   2.728856   5.067451
   26  H    5.944542   7.240474   6.780492   3.613168   5.970305
   27  H    5.919166   6.020438   6.099667   2.063258   4.422159
                 21         22         23         24         25
   21  H    0.000000
   22  H    2.502697   0.000000
   23  H    4.289801   2.428669   0.000000
   24  C    6.288707   4.974840   2.630039   0.000000
   25  H    6.733890   5.320131   2.986462   1.099522   0.000000
   26  H    5.990238   4.358994   1.972740   1.091567   1.766077
   27  H    7.188068   5.924444   3.589340   1.093873   1.766588
                 26         27
   26  H    0.000000
   27  H    1.750010   0.000000
Stoichiometry    C15H12
Framework group  C1[X(C15H12)]
Deg. of freedom    75
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -3.657593   -0.997269    0.022361
     2          6           0       -2.459425   -1.661517   -0.010757
```

This journal is © The Royal Society of Chemistry 2014

```
      3          6           0       -1.216879   -0.951125   -0.020494
      4          6           0       -1.224215    0.495444   -0.010888
      5          6           0       -2.503842    1.143664    0.031112
      6          6           0       -3.675045    0.427108    0.049163
      7          6           0        0.004229   -1.632469   -0.035359
      8          6           0       -0.000674    1.211472   -0.032371
      9          6           0        1.226306    0.502668   -0.010820
     10          6           0        1.221837   -0.945710   -0.021698
     11          6           0        2.465645   -1.654699   -0.013456
     12          1           0        2.437155   -2.742168   -0.029529
     13          6           0        3.663086   -0.990087    0.020674
     14          6           0        3.678359    0.434442    0.050527
     15          6           0        2.506995    1.149946    0.033545
     16          1           0        0.006982   -2.720934   -0.048816
     17          1           0       -4.593294   -1.550190    0.031959
     18          1           0       -2.430424   -2.749008   -0.025154
     19          1           0       -2.554524    2.226412    0.063711
     20          1           0       -4.626850    0.951054    0.086762
     21          1           0        4.599375   -1.541995    0.029392
     22          1           0        4.629301    0.959786    0.090103
     23          1           0        2.560743    2.232223    0.070046
     24          6           0       -0.019417    2.724906   -0.060892
     25          1           0       -0.142938    3.150178    0.945505
     26          1           0        0.898432    3.140485   -0.480849
     27          1           0       -0.840157    3.103520   -0.677006
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3935801      0.4479768
0.3398280
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9615121863 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
```

Supplementary Material (ESI) for Green Chemistry
This journal is © The Royal Society of Chemistry 2014

```
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860578217     A.U. after   12 cycles
             Convg  =    0.3808D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000157350    0.000152203   -0.000023982
      2        6           0.000113366   -0.000011084    0.000029102
      3        6           0.000186967   -0.000023977    0.000029571
```

4	6	-0.000075359	-0.000085662	-0.000040274
5	6	-0.000005355	0.000097425	0.000046160
6	6	-0.000022385	-0.000170218	0.000007485
7	6	-0.000035160	0.000060825	-0.000053524
8	6	-0.000105927	-0.000245672	-0.000022223
9	6	0.000244548	-0.000066507	-0.000046803
10	6	-0.000023660	-0.000209450	0.000033740
11	6	-0.000014019	-0.000056542	0.000023667
12	1	-0.000066675	-0.000018641	-0.000003321
13	6	-0.000098570	0.000189510	-0.000021014
14	6	0.000183655	-0.000081844	0.000003272
15	6	0.000033019	0.000226772	0.000032584
16	1	-0.000011462	0.000012476	0.000036592
17	1	-0.000082155	0.000035014	0.000026146
18	1	0.000044825	0.000049388	-0.000012497
19	1	0.000045037	-0.000067952	-0.000020200
20	1	-0.000009455	-0.000067194	-0.000024059
21	1	0.000009999	0.000089618	0.000019951
22	1	0.000071404	-0.000027379	-0.000026407
23	1	0.000098299	-0.000155528	-0.000049222
24	6	-0.000308542	0.000329640	-0.000072510
25	1	-0.000025424	-0.000007449	-0.000071829
26	1	-0.000101978	-0.000028464	0.000115819
27	1	0.000112357	0.000080688	0.000083775

Cartesian Forces: Max 0.000329640 RMS 0.000101804

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal Forces: Max 0.000499944 RMS 0.000087039
Search for a local minimum.
Step number 26 out of a maximum of 157
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 1 2 3 4
5
6 7 8 10
9
11 12 13 14
15
16 17 18 19
21
20 23 22 25
24
26
Use linear search instead of GDIIS.
Eigenvalues --- -0.00383 0.00001 0.01238 0.01617
0.01733

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.01816   0.01827   0.01836   0.01920
0.01976
     Eigenvalues ---    0.01982   0.01998   0.02022   0.02094
0.02104
     Eigenvalues ---    0.02126   0.02146   0.02210   0.02230
0.02277
     Eigenvalues ---    0.02326   0.02358   0.06565   0.06889
0.12328
     Eigenvalues ---    0.12777   0.15610   0.15862   0.15990
0.16000
     Eigenvalues ---    0.16000   0.16001   0.16003   0.16040
0.16186
     Eigenvalues ---    0.16294   0.21133   0.21998   0.22171
0.22622
     Eigenvalues ---    0.23042   0.23358   0.24452   0.24993
0.25265
     Eigenvalues ---    0.26654   0.31196   0.33525   0.33582
0.33627
     Eigenvalues ---    0.33631   0.33682   0.33682   0.33831
0.34003
     Eigenvalues ---    0.34140   0.34786   0.35692   0.37064
0.37160
     Eigenvalues ---    0.37593   0.38285   0.39308   0.39784
0.40468
     Eigenvalues ---    0.41117   0.42102   0.44381   0.45362
0.48492
     Eigenvalues ---    0.49535   0.49841   0.50466   0.51270
0.56048
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-3.83184802D-03 EMin=-3.83062314D-03
 RFO eigenvector is Hessian eigenvector with negative curvature.
 Taking step of  1.25D-01 in eigenvector direction.  Step.Grad= -
8.55D-06.
 Quartic linear search produced a step of  0.00601.
 Maximum step size (   0.050) exceeded in Quadratic search.
    -- Step size scaled by   0.400
 Iteration  1 RMS(Cart)=  0.00538185 RMS(Int)=  0.00002323
 Iteration  2 RMS(Cart)=  0.00004658 RMS(Int)=  0.00000771
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000771
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.58963   0.00017   0.00000   0.00131   0.00130
2.59094
    R2        2.69236  -0.00019   0.00000  -0.00142  -0.00142
2.69094
    R3        2.05394   0.00001   0.00000   0.00015   0.00015
2.05409
    R4        2.70480  -0.00002   0.00000   0.00019   0.00020
2.70500
    R5        2.05597  -0.00002   0.00000  -0.00062  -0.00062
2.05535
    R6        2.73371   0.00004   0.00000  -0.00024  -0.00023
2.73348
    R7        2.64262  -0.00011   0.00000  -0.00113  -0.00113
2.64148
    R8        2.71187   0.00006   0.00000  -0.00015  -0.00015
2.71172
    R9        2.67929   0.00014   0.00000  -0.00071  -0.00070
2.67859
   R10        2.59485   0.00009   0.00000  -0.00070  -0.00070
2.59415
   R11        2.04926  -0.00008   0.00000  -0.00016  -0.00016
2.04911
   R12        2.05439   0.00001   0.00000   0.00056   0.00056
2.05495
   R13        2.64183  -0.00011   0.00000  -0.00159  -0.00159
2.64023
   R14        2.05706  -0.00002   0.00000  -0.00028  -0.00028
2.05679
   R15        2.67805   0.00050   0.00000  -0.00205  -0.00205
2.67600
   R16        2.86070   0.00049  -0.00001   0.00494   0.00493
2.86563
   R17        2.73713   0.00009   0.00000  -0.00023  -0.00023
2.73690
```

This journal is © The Royal Society of Chemistry 2014

R18	2.71299	0.00024	0.00000	-0.00031	-0.00031
2.71269					
R19	2.70554	-0.00002	0.00000	0.00047	0.00047
2.70601					
R20	2.05595	-0.00002	0.00000	-0.00062	-0.00062
2.05532					
R21	2.58881	0.00012	0.00000	0.00132	0.00131
2.59013					
R22	2.69272	-0.00023	0.00000	-0.00112	-0.00112
2.69160					
R23	2.05391	0.00001	0.00000	0.00013	0.00013
2.05404					
R24	2.59404	0.00010	0.00000	-0.00085	-0.00085
2.59319					
R25	2.05437	0.00001	0.00000	0.00058	0.00058
2.05495					
R26	2.04889	-0.00018	0.00000	-0.00006	-0.00006
2.04883					
R27	2.07780	-0.00006	0.00000	0.00068	0.00068
2.07847					
R28	2.06276	-0.00012	0.00000	0.00014	0.00014
2.06290					
R29	2.06712	-0.00015	0.00000	0.00020	0.00020
2.06733					
A1	2.08951	0.00003	0.00000	0.00067	0.00066
2.09017					
A2	2.10173	0.00007	0.00000	0.00009	0.00009
2.10182					
A3	2.09194	-0.00011	0.00000	-0.00077	-0.00077
2.09117					
A4	2.11602	0.00001	0.00000	0.00018	0.00018
2.11620					
A5	2.10381	0.00006	0.00000	-0.00071	-0.00070
2.10311					
A6	2.06334	-0.00007	0.00000	0.00054	0.00054
2.06388					
A7	2.08502	-0.00004	0.00000	-0.00160	-0.00160
2.08342					
A8	2.11332	-0.00004	0.00000	0.00128	0.00127
2.11459					
A9	2.08485	0.00008	0.00000	0.00031	0.00032
2.08516					
A10	2.04474	0.00000	0.00000	0.00110	0.00107
2.04581					
A11	2.09500	-0.00001	0.00000	-0.00049	-0.00049
2.09451					
A12	2.14341	0.00001	0.00000	-0.00070	-0.00074
2.14266					
A13	2.12378	0.00003	0.00000	0.00025	0.00025
2.12402					
A14	2.08697	-0.00001	0.00000	-0.00004	-0.00004
2.08693					

This journal is © The Royal Society of Chemistry 2014

A15	2.07233	-0.00001	0.00000	-0.00019	-0.00019
2.07215					
A16	2.10716	-0.00003	0.00000	-0.00072	-0.00072
2.10644					
A17	2.08657	-0.00006	0.00000	0.00012	0.00012
2.08669					
A18	2.08946	0.00008	0.00000	0.00059	0.00060
2.09005					
A19	2.11892	0.00005	0.00000	-0.00035	-0.00036
2.11856					
A20	2.08234	-0.00003	0.00000	0.00018	0.00017
2.08251					
A21	2.08188	-0.00002	0.00000	0.00012	0.00011
2.08199					
A22	2.08788	-0.00010	0.00000	0.00020	0.00018
2.08806					
A23	2.08805	-0.00009	0.00000	-0.00045	-0.00050
2.08755					
A24	2.10719	0.00019	0.00001	0.00007	0.00002
2.10721					
A25	2.09134	-0.00008	0.00000	-0.00009	-0.00008
2.09127					
A26	2.14995	0.00018	0.00000	-0.00097	-0.00097
2.14898					
A27	2.04185	-0.00009	0.00000	0.00103	0.00102
2.04288					
A28	2.08747	0.00006	0.00000	0.00027	0.00027
2.08774					
A29	2.10999	-0.00005	0.00000	0.00134	0.00134
2.11133					
A30	2.08571	-0.00001	0.00000	-0.00162	-0.00162
2.08410					
A31	2.06252	-0.00009	0.00000	0.00038	0.00038
2.06290					
A32	2.11679	0.00004	0.00000	0.00028	0.00028
2.11707					
A33	2.10386	0.00005	0.00000	-0.00065	-0.00065
2.10321					
A34	2.08851	0.00005	0.00000	0.00053	0.00052
2.08903					
A35	2.10229	0.00007	0.00000	0.00024	0.00025
2.10254					
A36	2.09237	-0.00012	0.00000	-0.00077	-0.00077
2.09160					
A37	2.10794	-0.00002	0.00000	-0.00077	-0.00077
2.10717					
A38	2.08661	-0.00007	0.00000	0.00015	0.00015
2.08676					
A39	2.08863	0.00009	0.00000	0.00063	0.00063
2.08925					
A40	2.12539	0.00004	0.00000	0.00052	0.00052
2.12591					

This journal is © The Royal Society of Chemistry 2014

A41	2.08899	-0.00001	0.00000	-0.00008	-0.00008	2.08891
A42	2.06870	-0.00003	0.00000	-0.00040	-0.00040	2.06829
A43	1.95070	0.00000	0.00000	-0.00322	-0.00322	1.94748
A44	1.95785	0.00009	0.00001	0.00065	0.00066	1.95851
A45	1.94543	0.00008	0.00000	-0.00083	-0.00083	1.94460
A46	1.87481	-0.00007	0.00000	0.00257	0.00256	1.87737
A47	1.87274	-0.00006	0.00000	0.00114	0.00113	1.87387
A48	1.85712	-0.00006	0.00000	-0.00002	-0.00002	1.85710
D1	-0.00116	-0.00001	0.00000	-0.00354	-0.00354	-0.00471
D2	3.13483	0.00000	0.00000	-0.00147	-0.00148	3.13336
D3	-3.13884	0.00000	0.00000	0.00037	0.00037	-3.13847
D4	-0.00284	0.00001	0.00000	0.00244	0.00244	-0.00040
D5	0.00939	0.00000	0.00000	0.00167	0.00168	0.01107
D6	-3.12958	-0.00001	0.00000	0.00175	0.00175	-3.12783
D7	-3.13610	-0.00001	0.00000	-0.00222	-0.00221	-3.13831
D8	0.00811	-0.00002	0.00000	-0.00214	-0.00214	0.00598
D9	-0.01267	0.00001	0.00000	-0.00188	-0.00188	-0.01455
D10	3.12576	0.00000	0.00000	-0.00487	-0.00488	3.12089
D11	3.13439	0.00000	0.00000	-0.00390	-0.00390	3.13049
D12	-0.01036	-0.00001	0.00000	-0.00689	-0.00690	-0.01726
D13	0.01793	0.00000	0.00000	0.00883	0.00883	0.02676
D14	-3.13181	-0.00002	0.00000	-0.00390	-0.00391	-3.13572
D15	-3.12056	0.00001	0.00000	0.01177	0.01178	-3.10878
D16	0.01289	-0.00001	0.00000	-0.00096	-0.00096	0.01192
D17	-3.12212	0.00000	0.00000	0.00582	0.00583	-3.11629
D18	0.00975	-0.00001	0.00000	-0.00119	-0.00118	0.00856

This journal is © The Royal Society of Chemistry 2014

D19	0.01632	-0.00001	0.00000	0.00282	0.00282	0.01914
D20	-3.13501	-0.00002	0.00000	-0.00418	-0.00418	-3.13919
D21	-0.01017	-0.00002	0.00000	-0.01090	-0.01090	-0.02107
D22	3.11608	0.00000	0.00000	-0.00934	-0.00934	3.10673
D23	3.13982	0.00000	0.00000	0.00222	0.00221	-3.14116
D24	-0.01712	0.00002	0.00000	0.00378	0.00378	-0.01335
D25	-0.04255	0.00004	0.00000	-0.00242	-0.00242	-0.04497
D26	3.11210	0.00006	0.00000	0.01334	0.01333	3.12544
D27	3.09042	0.00002	0.00000	-0.01589	-0.01589	3.07453
D28	-0.03812	0.00004	0.00000	-0.00014	-0.00013	-0.03825
D29	-0.00342	0.00002	0.00000	0.00580	0.00580	0.00237
D30	3.13555	0.00002	0.00000	0.00572	0.00572	3.14127
D31	-3.12979	0.00000	0.00000	0.00425	0.00425	-3.12555
D32	0.00918	0.00000	0.00000	0.00417	0.00417	0.01335
D33	-0.01534	0.00001	0.00000	-0.00130	-0.00130	-0.01663
D34	3.12231	0.00001	0.00000	-0.00345	-0.00346	3.11885
D35	3.13598	0.00002	0.00000	0.00570	0.00571	-3.14149
D36	-0.00956	0.00002	0.00000	0.00355	0.00355	-0.00601
D37	0.04346	-0.00004	0.00000	0.00395	0.00395	0.04741
D38	-3.08852	-0.00004	0.00000	0.00663	0.00662	-3.08190
D39	-3.11134	-0.00007	0.00000	-0.01199	-0.01199	-3.12333
D40	0.03986	-0.00007	0.00000	-0.00931	-0.00931	0.03055
D41	1.44802	-0.00005	-0.00001	-0.00138	-0.00138	1.44664
D42	-2.72820	-0.00007	-0.00001	0.00010	0.00010	-2.72811
D43	-0.64761	-0.00003	0.00000	-0.00005	-0.00006	-0.64767
D44	-1.68036	-0.00002	0.00000	0.01455	0.01455	-1.66581

This journal is © The Royal Society of Chemistry 2014

D45	0.42660	-0.00005	0.00000	0.01604	0.01603	0.44262
D46	2.50719	0.00000	0.00000	0.01588	0.01587	2.52306
D47	-0.01487	0.00002	0.00000	-0.00213	-0.00213	-0.01700
D48	3.13062	0.00002	0.00000	-0.00001	-0.00001	3.13061
D49	3.11771	0.00002	0.00000	-0.00466	-0.00466	3.11305
D50	-0.01999	0.00002	0.00000	-0.00254	-0.00254	-0.02254
D51	-3.13904	0.00000	0.00000	0.00282	0.00282	-3.13622
D52	0.01911	-0.00003	0.00000	-0.00065	-0.00064	0.01846
D53	0.01190	0.00000	0.00000	0.00543	0.00543	0.01734
D54	-3.11313	-0.00003	0.00000	0.00197	0.00197	-3.11117
D55	0.01190	-0.00001	0.00000	0.00375	0.00375	0.01565
D56	-3.12388	-0.00002	0.00000	0.00095	0.00095	-3.12292
D57	-3.13364	0.00000	0.00000	0.00160	0.00160	-3.13203
D58	0.01377	-0.00002	0.00000	-0.00120	-0.00120	0.01257
D59	0.00152	0.00000	0.00000	0.00226	0.00226	0.00377
D60	3.13853	0.00000	0.00000	0.00108	0.00108	3.13961
D61	-3.13412	-0.00001	0.00000	-0.00061	-0.00061	-3.13474
D62	0.00289	-0.00001	0.00000	-0.00179	-0.00179	0.00110
D63	-0.01014	0.00001	0.00000	0.00058	0.00058	-0.00956
D64	3.12835	0.00002	0.00000	0.00114	0.00114	3.12949
D65	3.13600	0.00001	0.00000	0.00175	0.00175	3.13776
D66	-0.00869	0.00002	0.00000	0.00231	0.00231	-0.00638
D67	0.00307	-0.00001	0.00000	-0.00454	-0.00454	-0.00148
D68	3.12829	0.00001	0.00000	-0.00112	-0.00111	3.12718
D69	-3.13543	-0.00002	0.00000	-0.00510	-0.00510	-3.14052
D70	-0.01020	0.00001	0.00000	-0.00167	-0.00167	-0.01187

This journal is © The Royal Society of Chemistry 2014

```
         Item               Value     Threshold  Converged?
 Maximum Force            0.000500     0.000450     NO
 RMS     Force            0.000087     0.000300     YES
 Maximum Displacement     0.026672     0.001800     NO
 RMS     Displacement     0.005390     0.001200     NO
 Predicted change in Energy=-8.204197D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793558   -5.426124    0.014075
      2          6           0       -3.423230   -5.396414   -0.019685
      3          6           0       -2.707605   -4.156859   -0.038501
      4          6           0       -3.444541   -2.912161   -0.039914
      5          6           0       -4.876071   -2.996959    0.012128
      6          6           0       -5.526624   -4.205536    0.036759
      7          6           0       -1.310110   -4.128665   -0.048154
      8          6           0       -2.749667   -1.676992   -0.065654
      9          6           0       -1.333952   -1.669195   -0.034558
     10          6           0       -0.606605   -2.921613   -0.036344
     11          6           0        0.825124   -2.903308   -0.018459
     12          1           0        1.351395   -3.855076   -0.029309
     13          6           0        1.521786   -1.723400    0.015062
     14          6           0        0.814889   -0.487065    0.037297
     15          6           0       -0.556967   -0.463149    0.014267
     16          1           0       -0.758108   -5.066703   -0.049347
     17          1           0       -5.323323   -6.375114    0.030964
     18          1           0       -2.851116   -6.321378   -0.029564
     19          1           0       -5.465177   -2.087224    0.045762
     20          1           0       -6.612986   -4.232890    0.076528
     21          1           0        2.608629   -1.725329    0.030163
     22          1           0        1.369568    0.447490    0.075321
     23          1           0       -1.058312    0.497640    0.046117
     24          6           0       -3.531507   -0.377849   -0.088218
     25          1           0       -3.845596   -0.077084    0.922043
     26          1           0       -2.952548    0.444961   -0.511858
     27          1           0       -4.435220   -0.466016   -0.698402
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1          2          3          4          5
    1  C    0.000000
    2  C    1.371065   0.000000
    3  C    2.442334   1.431422   0.000000
    4  C    2.853554   2.484427   1.446497   0.000000
    5  C    2.430566   2.805199   2.459711   1.434983   0.000000
    6  C    1.423986   2.417776   2.820444   2.452298   1.372765
    7  C    3.717752   2.464402   1.397813   2.456776   3.741720
```

This journal is © The Royal Society of Chemistry 2014

8	C	4.270812	3.780198	2.480373	1.417447	2.503988
9	C	5.107421	4.272875	2.841727	2.449404	3.783086
10	C	4.879107	3.749439	2.437219	2.837954	4.270405
11	C	6.159159	4.925860	3.748595	4.269729	5.702046
12	H	6.342753	5.017256	4.070214	4.887761	6.286447
13	C	7.320774	6.159986	4.879789	5.106915	6.523383
14	C	7.473253	6.485877	5.087347	4.902020	6.219906
15	C	6.525322	5.705586	4.274520	3.786645	5.007480
16	H	4.051921	2.685604	2.151389	3.443700	4.609256
17	H	1.086977	2.137936	3.430373	3.940418	3.407686
18	H	2.139267	1.087645	2.169289	3.460495	3.892806
19	H	3.405926	3.889032	3.448869	2.184223	1.084341
20	H	2.176701	3.396702	3.907815	3.434666	2.132732
21	H	8.275778	7.061350	5.846315	6.168821	7.591976
22	H	8.513942	7.558515	6.151124	5.871642	7.132757
23	H	7.003147	6.351145	4.938795	4.162719	5.175777
24	C	5.204643	5.020200	3.868101	2.536263	2.945787
25	H	5.507746	5.418534	4.343067	3.020574	3.227305
26	H	6.175400	5.880938	4.632582	3.425646	3.977602
27	H	5.023813	5.078740	4.128250	2.720050	2.665497

		6	7	8	9	10
6	C	0.000000				
7	C	4.218070	0.000000			
8	C	3.757062	2.843120	0.000000		
9	C	4.900674	2.459624	1.416077	0.000000	
10	C	5.085311	1.397152	2.478437	1.448305	0.000000
11	C	6.484100	2.462033	3.779578	2.486947	1.431958
12	H	6.887259	2.675596	4.643714	3.462542	2.169140
13	C	7.472720	3.716037	4.272467	2.856683	2.443032
14	C	7.351314	4.217128	3.759333	2.453592	2.820123
15	C	6.221210	3.742610	2.507536	1.435492	2.459485
16	H	4.846418	1.088404	3.931503	3.445995	2.150473
17	H	2.179091	4.599856	5.357741	6.169688	5.846249
18	H	3.411676	2.680119	4.645634	4.893324	4.073853
19	H	2.119222	4.630431	2.748582	4.153097	4.930382
20	H	1.087434	5.305366	4.634444	5.869674	6.148886
21	H	8.504928	4.597681	5.359370	3.943512	3.431217
22	H	8.319230	5.304443	4.636959	3.435324	3.907504
23	H	6.487354	4.634111	2.757208	2.185786	3.449946
24	C	4.318251	4.359453	1.516428	2.549450	3.876657
25	H	4.544634	4.877015	2.176307	3.123820	4.415983
26	H	5.343591	4.881668	2.177830	2.705055	4.130784
27	H	3.964294	4.858408	2.169775	3.392077	4.596364

		11	12	13	14	15
11	C	0.000000				
12	H	1.087631	0.000000			
13	C	1.370637	2.138936	0.000000		
14	C	2.416908	3.411124	1.424331	0.000000	
15	C	2.804571	3.892160	2.430934	1.372258	0.000000
16	H	2.681018	2.432785	4.047189	4.843027	4.608385
17	H	7.061110	7.134850	8.276123	8.505693	7.594061
18	H	5.019768	4.872756	6.345523	6.890811	6.291573

This journal is © The Royal Society of Chemistry 2014

19	H	6.343344	7.042485	6.996496	6.480727	5.170024
20	H	7.556606	7.974040	8.513274	8.319019	7.133736
21	H	2.137963	2.473862	1.086950	2.179645	3.407983
22	H	3.396036	4.303876	2.177054	1.087432	2.131789
23	H	3.888181	4.975793	3.404539	2.116271	1.084194
24	C	5.036173	5.994773	5.230386	4.349579	2.977527
25	H	5.539649	6.495152	5.686981	4.761405	3.433393
26	H	5.071997	6.103040	4.999909	3.919672	2.615393
27	H	5.837288	6.739312	6.129923	5.301447	3.943191

		16	17	18	19	20
16	H	0.000000				
17	H	4.749692	0.000000			
18	H	2.440345	2.473531	0.000000		
19	H	5.571611	4.290262	4.976651	0.000000	
20	H	5.915293	2.500886	4.304034	2.433576	0.000000
21	H	4.744051	9.194365	7.136949	8.081928	9.556579
22	H	5.911757	9.557441	7.977641	7.289677	9.253493
23	H	5.573253	8.088591	7.051162	5.109010	7.296112
24	C	5.447807	6.260351	5.982634	2.584375	4.938015
25	H	5.947477	6.530152	6.394197	2.726092	5.063998
26	H	5.950456	7.240763	6.784264	3.610569	5.968861
27	H	5.925263	6.019812	6.102622	2.059832	4.419561

		21	22	23	24	25
21	H	0.000000				
22	H	2.501691	0.000000			
23	H	4.288158	2.428573	0.000000		
24	C	6.287367	4.972772	2.627017	0.000000	
25	H	6.720802	5.309430	2.977668	1.099881	0.000000
26	H	5.994217	4.361820	1.975409	1.091642	1.768089
27	H	7.192530	5.926947	3.589770	1.093982	1.767702

		26	27
26	H	0.000000	
27	H	1.750141	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.657598	-0.995039	0.026477
2	6	0	-2.459805	-1.661172	-0.010661
3	6	0	-1.216208	-0.952521	-0.026467
4	6	0	-1.223788	0.493946	-0.021147
5	6	0	-2.502220	1.143347	0.034214
6	6	0	-3.674007	0.428551	0.055789
7	6	0	0.004275	-1.633793	-0.039573
8	6	0	-0.000318	1.209320	-0.043841

```
      9          6           0        1.225600    0.501054   -0.016324
     10          6           0        1.221005   -0.947218   -0.024848
     11          6           0        2.466050   -1.654440   -0.010542
     12          1           0        2.439706   -2.741636   -0.026446
     13          6           0        3.663173   -0.987941    0.025804
     14          6           0        3.677303    0.436028    0.054663
     15          6           0        2.505256    1.149484    0.035223
     16          1           0        0.007076   -2.722175   -0.045831
     17          1           0       -4.594050   -1.546731    0.041015
     18          1           0       -2.433044   -2.748385   -0.025606
     19          1           0       -2.551332    2.225885    0.072897
     20          1           0       -4.625504    0.953303    0.098221
     21          1           0        4.600311   -1.538468    0.038126
     22          1           0        4.627984    0.962425    0.094917
     23          1           0        2.557675    2.231782    0.072099
     24          6           0       -0.019171    2.725552   -0.059344
     25          1           0       -0.138173    3.139050    0.952880
     26          1           0        0.895935    3.145386   -0.481247
     27          1           0       -0.843872    3.108613   -0.667562
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3936966      0.4481253
0.3399440
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       879.0496159035 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860548291     A.U. after   11 cycles
             Convg  =    0.3414D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000519989   -0.000353647    0.000078735
      2        6          -0.000451437    0.000074756   -0.000258180
      3        6          -0.000753124   -0.000258258   -0.000185334
      4        6          -0.000157982    0.000052253    0.000927926
      5        6           0.000008745    0.000355537   -0.000625202
      6        6          -0.000413578   -0.000113711    0.000038534
      7        6           0.000154138   -0.000453341    0.000112923
      8        6          -0.001294973    0.001061607    0.000921005
      9        6           0.000565872    0.000099820   -0.000127580
```

```
     10        6           0.000760214    0.000575317   -0.000013742
     11        6           0.000154587    0.000491433   -0.000186139
     12        1           0.000014962   -0.000233649    0.000071974
     13        6          -0.000081539   -0.000614481    0.000006536
     14        6           0.000400753    0.000205983    0.000097654
     15        6          -0.000219147    0.000508035   -0.000372374
     16        1           0.000035308   -0.000089942   -0.000145167
     17        1           0.000033564    0.000016430   -0.000057513
     18        1           0.000197491   -0.000120170    0.000081386
     19        1           0.000043453   -0.000034942   -0.000186514
     20        1           0.000199165   -0.000032921    0.000137568
     21        1          -0.000027808   -0.000030629   -0.000018367
     22        1          -0.000060278   -0.000199173    0.000095625
     23        1           0.000024803   -0.000170858   -0.000101644
     24        6           0.000135685   -0.000928867   -0.000314183
     25        1           0.000068139    0.000114511   -0.000411803
     26        1          -0.000062888   -0.000069125    0.000244328
     27        1           0.000205886    0.000148034    0.000189548
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.001294973 RMS     0.000370390


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.001254796 RMS     0.000224386
 Search for a local minimum.
 Step number  27 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
21
                                                     20   23   22   25
24
                                                     26   27
 DE=  2.99D-05 DEPred=-8.20D-06 R=-3.65D+00
 Trust test=-3.65D+00 RLast= 5.00D-02 DXMaxT set to 5.00D-02
     Eigenvalues ---   -0.05370   0.00000   0.01536   0.01678
0.01809
     Eigenvalues ---    0.01818   0.01822   0.01863   0.01976
0.01981
     Eigenvalues ---    0.01997   0.02008   0.02081   0.02101
0.02118
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02146   0.02196   0.02230   0.02235
0.02294
     Eigenvalues ---    0.02357   0.02589   0.06066   0.06848
0.07592
     Eigenvalues ---    0.12518   0.14903   0.15958   0.15995
0.15999
     Eigenvalues ---    0.16000   0.16002   0.16009   0.16024
0.16178
     Eigenvalues ---    0.16336   0.21276   0.22001   0.22132
0.22618
     Eigenvalues ---    0.23185   0.23346   0.24346   0.24602
0.24998
     Eigenvalues ---    0.26561   0.29873   0.31631   0.33441
0.33614
     Eigenvalues ---    0.33631   0.33671   0.33682   0.33683
0.33816
     Eigenvalues ---    0.34018   0.34115   0.35714   0.36966
0.37207
     Eigenvalues ---    0.37431   0.38195   0.39221   0.39833
0.40489
     Eigenvalues ---    0.41129   0.42018   0.43150   0.45332
0.46657
     Eigenvalues ---    0.49539   0.49841   0.51265   0.51922
0.55746
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is  -5.37D-02 should be greater than     0.000000
Eigenvector:
                           D40       D38       A43       D39       D28
   1                     0.25917   0.24725   0.23670   0.22019  -
0.21875
                           D26       D37       D27       D25       R16
   1                    -0.21659   0.20827  -0.20656  -0.20440  -
0.17571
 Eigenvalue     2 is   3.33D-06 Eigenvector:
                           D44       D41       D46       D45       D43
   1                     0.42705   0.40649   0.40452   0.40324
0.38395
                           D42       D40       D39       D28       D26
   1                     0.38268  -0.06304  -0.05755   0.05395
0.05365
 Use linear search instead of GDIIS.
 RFO step:  Lambda=-2.67128557D-05 EMin= 5.37018192D-02
 Quartic linear search produced a step of -0.94859.
 Maximum step size (   0.050) exceeded in Quadratic search.
    -- Step size scaled by   0.126
 Iteration  1 RMS(Cart)=  0.00860986 RMS(Int)=  0.00009910
 Iteration  2 RMS(Cart)=  0.00011486 RMS(Int)=  0.00000259
 Iteration  3 RMS(Cart)=  0.00000001 RMS(Int)=  0.00000259
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.59094  -0.00048  -0.00124   0.00013  -0.00111
2.58983
    R2        2.69094   0.00033   0.00134  -0.00013   0.00122
2.69216
    R3        2.05409  -0.00003  -0.00014   0.00007  -0.00007
2.05402
    R4        2.70500  -0.00008  -0.00019  -0.00017  -0.00036
2.70464
    R5        2.05535   0.00021   0.00059   0.00007   0.00066
2.05601
    R6        2.73348   0.00027   0.00022  -0.00038  -0.00016
2.73332
    R7        2.64148   0.00045   0.00108   0.00015   0.00122
2.64270
    R8        2.71172   0.00008   0.00014  -0.00024  -0.00011
2.71162
    R9        2.67859   0.00057   0.00067   0.00010   0.00077
2.67935
   R10        2.59415   0.00051   0.00066   0.00016   0.00082
2.59497
   R11        2.04911  -0.00006   0.00015   0.00015   0.00029
2.04940
   R12        2.05495  -0.00019  -0.00053   0.00004  -0.00049
2.05446
```

This journal is © The Royal Society of Chemistry 2014

R13	2.64023	0.00055	0.00151	-0.00003	0.00148
2.64172					
R14	2.05679	0.00010	0.00026	0.00006	0.00033
2.05711					
R15	2.67600	0.00125	0.00195	-0.00018	0.00177
2.67776					
R16	2.86563	-0.00080	-0.00468	-0.00015	-0.00483
2.86081					
R17	2.73690	0.00028	0.00022	0.00026	0.00047
2.73737					
R18	2.71269	0.00032	0.00029	-0.00002	0.00027
2.71296					
R19	2.70601	-0.00014	-0.00045	-0.00002	-0.00047
2.70554					
R20	2.05532	0.00021	0.00059	0.00007	0.00066
2.05598					
R21	2.59013	-0.00056	-0.00125	-0.00003	-0.00128
2.58885					
R22	2.69160	0.00026	0.00106	-0.00005	0.00102
2.69261					
R23	2.05404	-0.00003	-0.00012	0.00007	-0.00005
2.05399					
R24	2.59319	0.00055	0.00081	0.00000	0.00081
2.59400					
R25	2.05495	-0.00020	-0.00055	0.00004	-0.00051
2.05444					
R26	2.04883	-0.00017	0.00006	0.00008	0.00014
2.04897					
R27	2.07847	-0.00036	-0.00064	-0.00013	-0.00078
2.07770					
R28	2.06290	-0.00018	-0.00013	-0.00045	-0.00058
2.06232					
R29	2.06733	-0.00029	-0.00019	0.00032	0.00013
2.06745					
A1	2.09017	-0.00007	-0.00063	0.00019	-0.00044
2.08973					
A2	2.10182	0.00001	-0.00008	-0.00038	-0.00047
2.10135					
A3	2.09117	0.00006	0.00073	0.00020	0.00093
2.09210					
A4	2.11620	0.00002	-0.00017	-0.00007	-0.00023
2.11596					
A5	2.10311	0.00010	0.00067	-0.00021	0.00046
2.10356					
A6	2.06388	-0.00012	-0.00051	0.00028	-0.00023
2.06365					
A7	2.08342	0.00035	0.00152	-0.00021	0.00131
2.08473					
A8	2.11459	-0.00039	-0.00120	0.00048	-0.00073
2.11386					
A9	2.08516	0.00003	-0.00030	-0.00027	-0.00057
2.08460					

This journal is © The Royal Society of Chemistry 2014

A10	2.04581	-0.00029	-0.00101	0.00047	-0.00054
2.04527					
A11	2.09451	0.00001	0.00047	0.00033	0.00080
2.09531					
A12	2.14266	0.00029	0.00070	-0.00080	-0.00009
2.14257					
A13	2.12402	-0.00010	-0.00023	-0.00022	-0.00045
2.12357					
A14	2.08693	0.00003	0.00004	-0.00021	-0.00017
2.08676					
A15	2.07215	0.00007	0.00018	0.00042	0.00060
2.07275					
A16	2.10644	0.00009	0.00068	-0.00017	0.00051
2.10695					
A17	2.08669	-0.00009	-0.00012	0.00026	0.00015
2.08684					
A18	2.09005	-0.00001	-0.00057	-0.00009	-0.00066
2.08939					
A19	2.11856	0.00016	0.00034	-0.00001	0.00033
2.11889					
A20	2.08251	-0.00010	-0.00016	0.00005	-0.00011
2.08240					
A21	2.08199	-0.00007	-0.00010	-0.00003	-0.00014
2.08185					
A22	2.08806	-0.00007	-0.00018	-0.00001	-0.00018
2.08788					
A23	2.08755	0.00006	0.00047	-0.00173	-0.00126
2.08629					
A24	2.10721	0.00001	-0.00002	0.00176	0.00173
2.10894					
A25	2.09127	-0.00008	0.00007	-0.00032	-0.00025
2.09102					
A26	2.14898	0.00041	0.00092	0.00038	0.00130
2.15028					
A27	2.04288	-0.00032	-0.00097	-0.00006	-0.00103
2.04184					
A28	2.08774	-0.00005	-0.00026	0.00021	-0.00005
2.08769					
A29	2.11133	-0.00032	-0.00127	-0.00012	-0.00139
2.10995					
A30	2.08410	0.00037	0.00153	-0.00009	0.00144
2.08554					
A31	2.06290	-0.00012	-0.00036	0.00011	-0.00025
2.06265					
A32	2.11707	0.00003	-0.00026	0.00008	-0.00018
2.11689					
A33	2.10321	0.00009	0.00061	-0.00020	0.00042
2.10363					
A34	2.08903	0.00000	-0.00050	0.00001	-0.00049
2.08854					
A35	2.10254	-0.00003	-0.00023	-0.00027	-0.00051
2.10203					

This journal is © The Royal Society of Chemistry 2014

A36	2.09160	0.00003	0.00073	0.00027	0.00100
2.09260					
A37	2.10717	0.00009	0.00073	-0.00003	0.00070
2.10787					
A38	2.08676	-0.00010	-0.00014	0.00028	0.00014
2.08690					
A39	2.08925	0.00000	-0.00059	-0.00025	-0.00084
2.08841					
A40	2.12591	-0.00017	-0.00050	0.00008	-0.00042
2.12549					
A41	2.08891	0.00002	0.00007	0.00015	0.00022
2.08913					
A42	2.06829	0.00015	0.00038	-0.00023	0.00015
2.06844					
A43	1.94748	0.00025	0.00305	0.00065	0.00371
1.95119					
A44	1.95851	-0.00005	-0.00062	0.00093	0.00031
1.95881					
A45	1.94460	0.00018	0.00079	-0.00140	-0.00061
1.94399					
A46	1.87737	-0.00022	-0.00243	-0.00006	-0.00249
1.87488					
A47	1.87387	-0.00016	-0.00108	-0.00048	-0.00156
1.87231					
A48	1.85710	-0.00003	0.00002	0.00033	0.00035
1.85745					
D1	-0.00471	0.00010	0.00336	-0.00011	0.00325	-
0.00146					
D2	3.13336	0.00005	0.00140	-0.00026	0.00114
3.13450					
D3	-3.13847	0.00002	-0.00035	-0.00017	-0.00052	-
3.13899					
D4	-0.00040	-0.00003	-0.00231	-0.00031	-0.00263	-
0.00303					
D5	0.01107	-0.00003	-0.00159	0.00037	-0.00122
0.00985					
D6	-3.12783	-0.00004	-0.00166	0.00061	-0.00105	-
3.12888					
D7	-3.13831	0.00005	0.00210	0.00042	0.00252	-
3.13579					
D8	0.00598	0.00004	0.00203	0.00067	0.00270
0.00867					
D9	-0.01455	0.00001	0.00178	-0.00025	0.00153	-
0.01302					
D10	3.12089	0.00008	0.00463	-0.00020	0.00442
3.12531					
D11	3.13049	0.00005	0.00370	-0.00011	0.00359
3.13408					
D12	-0.01726	0.00012	0.00654	-0.00006	0.00648	-
0.01078					
D13	0.02676	-0.00018	-0.00838	0.00037	-0.00801
0.01875					

This journal is © The Royal Society of Chemistry 2014

D14	-3.13572	0.00012	0.00371	0.00029	0.00400	-3.13172
D15	-3.10878	-0.00025	-0.01117	0.00032	-0.01085	-3.11964
D16	0.01192	0.00005	0.00091	0.00023	0.00115	0.01307
D17	-3.11629	-0.00017	-0.00553	0.00080	-0.00473	-3.12102
D18	0.00856	0.00001	0.00112	0.00092	0.00204	0.01060
D19	0.01914	-0.00010	-0.00268	0.00085	-0.00183	0.01731
D20	-3.13919	0.00008	0.00397	0.00097	0.00494	-3.13425
D21	-0.02107	0.00027	0.01034	-0.00013	0.01022	-0.01086
D22	3.10673	0.00021	0.00886	-0.00045	0.00841	3.11515
D23	-3.14116	-0.00004	-0.00210	-0.00005	-0.00215	3.13988
D24	-0.01335	-0.00009	-0.00358	-0.00038	-0.00395	-0.01730
D25	-0.04497	0.00006	0.00230	-0.00151	0.00078	-0.04419
D26	3.12544	-0.00022	-0.01265	-0.00252	-0.01515	3.11028
D27	3.07453	0.00037	0.01507	-0.00158	0.01348	3.08801
D28	-0.03825	0.00009	0.00012	-0.00259	-0.00246	-0.04071
D29	0.00237	-0.00016	-0.00550	-0.00025	-0.00574	-0.00337
D30	3.14127	-0.00015	-0.00543	-0.00049	-0.00592	3.13535
D31	-3.12555	-0.00011	-0.00403	0.00008	-0.00395	-3.12950
D32	0.01335	-0.00010	-0.00395	-0.00017	-0.00412	0.00923
D33	-0.01663	0.00005	0.00123	-0.00064	0.00059	-0.01605
D34	3.11885	0.00012	0.00328	-0.00071	0.00257	3.12142
D35	-3.14149	-0.00013	-0.00541	-0.00076	-0.00618	3.13551
D36	-0.00601	-0.00006	-0.00337	-0.00083	-0.00420	-0.01021
D37	0.04741	-0.00012	-0.00375	0.00170	-0.00205	0.04537
D38	-3.08190	-0.00021	-0.00628	0.00194	-0.00435	-3.08625
D39	-3.12333	0.00017	0.01137	0.00266	0.01405	-3.10927

This journal is © The Royal Society of Chemistry 2014

D40	0.03055	0.00008	0.00884	0.00290	0.01175	0.04230
D41	1.44664	0.00019	0.00131	-0.02035	-0.01904	1.42760
D42	-2.72811	0.00004	-0.00009	-0.01930	-0.01940	-2.74750
D43	-0.64767	0.00010	0.00005	-0.01922	-0.01916	-0.66683
D44	-1.66581	-0.00010	-0.01380	-0.02134	-0.03514	-1.70095
D45	0.44262	-0.00025	-0.01520	-0.02030	-0.03550	0.40713
D46	2.52306	-0.00019	-0.01506	-0.02021	-0.03526	2.48780
D47	-0.01700	0.00006	0.00202	-0.00065	0.00138	-0.01562
D48	3.13061	-0.00001	0.00001	-0.00058	-0.00057	3.13004
D49	3.11305	0.00015	0.00442	-0.00087	0.00355	3.11660
D50	-0.02254	0.00008	0.00241	-0.00080	0.00161	-0.02092
D51	-3.13622	-0.00007	-0.00268	0.00025	-0.00243	-3.13865
D52	0.01846	0.00000	0.00061	0.00076	0.00137	0.01984
D53	0.01734	-0.00016	-0.00515	0.00048	-0.00468	0.01266
D54	-3.11117	-0.00009	-0.00187	0.00099	-0.00087	-3.11204
D55	0.01565	-0.00010	-0.00356	0.00040	-0.00317	0.01249
D56	-3.12292	-0.00004	-0.00090	0.00056	-0.00035	-3.12327
D57	-3.13203	-0.00003	-0.00152	0.00033	-0.00119	-3.13323
D58	0.01257	0.00003	0.00113	0.00049	0.00163	0.01420
D59	0.00377	-0.00007	-0.00214	0.00018	-0.00196	0.00181
D60	3.13961	-0.00004	-0.00102	0.00013	-0.00089	3.13871
D61	-3.13474	-0.00001	0.00058	0.00034	0.00092	-3.13381
D62	0.00110	0.00002	0.00170	0.00029	0.00199	0.00309
D63	-0.00956	0.00000	-0.00055	-0.00052	-0.00107	-0.01063
D64	3.12949	0.00000	-0.00108	-0.00087	-0.00195	3.12754
D65	3.13776	-0.00003	-0.00166	-0.00047	-0.00213	3.13562

This journal is © The Royal Society of Chemistry 2014

```
   D66       -0.00638  -0.00003  -0.00219  -0.00082  -0.00301  -
0.00939
   D67       -0.00148   0.00012   0.00431   0.00018   0.00449
0.00301
   D68        3.12718   0.00004   0.00106  -0.00033   0.00073
3.12791
   D69       -3.14052   0.00012   0.00484   0.00053   0.00537  -
3.13516
   D70       -0.01187   0.00004   0.00158   0.00003   0.00161  -
0.01026
         Item               Value     Threshold  Converged?
 Maximum Force            0.001255     0.000450     NO
 RMS     Force            0.000224     0.000300     YES
 Maximum Displacement     0.057046     0.001800     NO
 RMS     Displacement     0.008607     0.001200     NO
 Predicted change in Energy=-3.342795D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792764   -5.426694    0.014461
      2          6           0       -3.423008   -5.395898   -0.017685
      3          6           0       -2.708636   -4.155771   -0.031297
      4          6           0       -3.445059   -2.910873   -0.027171
      5          6           0       -4.876832   -2.996288    0.014623
      6          6           0       -5.526619   -4.205819    0.036678
      7          6           0       -1.310531   -4.127260   -0.044616
      8          6           0       -2.750604   -1.674998   -0.052634
      9          6           0       -1.333836   -1.666949   -0.027659
     10          6           0       -0.606457   -2.919626   -0.033408
     11          6           0        0.825121   -2.903482   -0.022457
     12          1           0        1.349823   -3.856492   -0.035071
     13          6           0        1.523140   -1.725133    0.010011
     14          6           0        0.817124   -0.487743    0.035717
     15          6           0       -0.555170   -0.461610    0.015802
     16          1           0       -0.758420   -5.065382   -0.054665
     17          1           0       -5.321415   -6.376335    0.026892
     18          1           0       -2.849567   -6.320441   -0.028277
     19          1           0       -5.466487   -2.086576    0.044056
     20          1           0       -6.612795   -4.233405    0.074180
     21          1           0        2.610003   -1.729080    0.020647
     22          1           0        1.372433    0.446081    0.074751
     23          1           0       -1.055079    0.499943    0.049558
     24          6           0       -3.533382   -0.379723   -0.089241
     25          1           0       -3.875783   -0.081244    0.912011
     26          1           0       -2.945963    0.446443   -0.493462
     27          1           0       -4.420667   -0.467658   -0.723225
```

This journal is © The Royal Society of Chemistry 2014

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370478	0.000000			
3	C	2.441501	1.431233	0.000000		
4	C	2.854364	2.485140	1.446412	0.000000	
5	C	2.431860	2.805847	2.459184	1.434927	0.000000
6	C	1.424631	2.417524	2.819247	2.452315	1.373199
7	C	3.717252	2.464291	1.398459	2.456850	3.741806
8	C	4.272018	3.781328	2.481220	1.417852	2.504231
9	C	5.108976	4.274319	2.843294	2.450431	3.784409
10	C	4.879840	3.750350	2.438691	2.838622	4.271333
11	C	6.158619	4.925319	3.749099	4.270189	5.702829
12	H	6.340297	5.014977	4.069481	4.887244	6.285989
13	C	7.320670	6.159518	4.880331	5.107873	6.524990
14	C	7.474257	6.486259	5.088211	4.903235	6.222087
15	C	6.527577	5.707260	4.276267	3.788430	5.010126
16	H	4.051080	2.685263	2.152040	3.443935	4.609476
17	H	1.086942	2.137098	3.429417	3.941200	3.409182
18	H	2.139304	1.087992	2.169255	3.461180	3.893795
19	H	3.407516	3.889888	3.448621	2.184195	1.084497
20	H	2.177158	3.396257	3.906355	3.434226	2.132504
21	H	8.274862	7.060046	5.846319	6.169497	7.593323
22	H	8.514856	7.558672	6.151700	5.872629	7.134903
23	H	7.006892	6.353939	4.941301	4.165520	5.179830
24	C	5.202760	5.017899	3.865501	2.533451	2.943137
25	H	5.497298	5.414322	4.342100	3.012373	3.210122
26	H	6.177572	5.881061	4.631446	3.426091	3.979799
27	H	5.027392	5.077465	4.124560	2.721324	2.673289

		6	7	8	9	10
6	C	0.000000				
7	C	4.217604	0.000000			
8	C	3.757564	2.843847	0.000000		
9	C	4.901982	2.460480	1.417011	0.000000	
10	C	5.085980	1.397936	2.479281	1.448556	0.000000
11	C	6.484148	2.461531	3.780992	2.487999	1.431711
12	H	6.885683	2.674115	4.644645	3.463550	2.169044
13	C	7.473527	3.715224	4.274498	2.857817	2.442107
14	C	7.353037	4.216568	3.761125	2.453807	2.818761
15	C	6.223732	3.743156	2.509368	1.435637	2.459044
16	H	4.845917	1.088577	3.932366	3.446909	2.151235
17	H	2.180217	4.598982	5.358914	6.171067	5.846648
18	H	3.412104	2.679355	4.646561	4.894123	4.073955
19	H	2.120108	4.630791	2.748593	4.154519	4.931517
20	H	1.087173	5.304657	4.634440	5.870644	6.149283
21	H	8.505240	4.596315	5.361381	3.944624	3.430151
22	H	8.320970	5.303583	4.638388	3.435008	3.905854
23	H	6.491458	4.635206	2.759641	2.186112	3.449869
24	C	4.316000	4.357418	1.513875	2.549263	3.875708
25	H	4.528088	4.885274	2.176377	3.139894	4.431560
26	H	5.346436	4.877998	2.175547	2.698583	4.124968

27	H	3.971703	4.850376	2.167134	3.383879	4.586523
		11	12	13	14	15
11	C	0.000000				
12	H	1.087979	0.000000			
13	C	1.369960	2.138869	0.000000		
14	C	2.416452	3.411340	1.424869	0.000000	
15	C	2.805246	3.893174	2.432261	1.372686	0.000000
16	H	2.680010	2.430328	4.045611	4.842033	4.608795
17	H	7.059961	7.131540	8.275379	8.506306	7.596130
18	H	5.017866	4.868879	6.343414	6.889781	6.292226
19	H	6.344769	7.042794	6.999049	6.483833	5.173234
20	H	7.556495	7.972282	8.514046	8.320766	7.136152
21	H	2.137026	2.473265	1.086922	2.180725	3.409519
22	H	3.395376	4.304033	2.177401	1.087162	2.131439
23	H	3.888913	4.976870	3.405839	2.116804	1.084266
24	C	5.036900	5.994709	5.233392	4.353640	2.981189
25	H	5.562082	6.515859	5.715273	4.791295	3.460396
26	H	5.066055	6.097470	4.994207	3.913253	2.607643
27	H	5.826029	6.727281	6.119455	5.292528	3.935514
		16	17	18	19	20
16	H	0.000000				
17	H	4.748280	0.000000			
18	H	2.439009	2.473094	0.000000		
19	H	5.572156	4.292245	4.977862	0.000000	
20	H	5.914599	2.502408	4.304428	2.433886	0.000000
21	H	4.741609	9.192628	7.133716	8.084432	9.556909
22	H	5.910458	9.557994	7.976323	7.292882	9.255347
23	H	5.574200	8.092300	7.052935	5.113768	7.300232
24	C	5.445824	6.258586	5.980255	2.582249	4.935621
25	H	5.957688	6.519314	6.392562	2.702784	5.043177
26	H	5.946268	7.243192	6.783540	3.613607	5.972340
27	H	5.915918	6.023826	6.099703	2.074452	4.429686
		21	22	23	24	25
21	H	0.000000				
22	H	2.503164	0.000000			
23	H	4.289779	2.428241	0.000000		
24	C	6.290788	4.977536	2.633450	0.000000	
25	H	6.750949	5.340679	3.006322	1.099470	0.000000
26	H	5.988820	4.355618	1.968038	1.091332	1.765892
27	H	7.181564	5.918758	3.586172	1.094049	1.766412
		26	27			
26	H	0.000000				
27	H	1.750179	0.000000			

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

This journal is © The Royal Society of Chemistry 2014

Number	Number	Type	X	Y	Z
1	6	0	-3.657086	-0.997516	0.023386
2	6	0	-2.458978	-1.662019	-0.011056
3	6	0	-1.216422	-0.951824	-0.021380
4	6	0	-1.223986	0.494534	-0.011398
5	6	0	-2.503201	1.143140	0.032602
6	6	0	-3.674561	0.426733	0.051367
7	6	0	0.005001	-1.632682	-0.037053
8	6	0	-0.000768	1.211157	-0.033553
9	6	0	1.226429	0.503061	-0.011041
10	6	0	1.222260	-0.945442	-0.022659
11	6	0	2.466333	-1.653966	-0.014167
12	1	0	2.438410	-2.741454	-0.031196
13	6	0	3.663580	-0.989040	0.021391
14	6	0	3.678471	0.435404	0.052872
15	6	0	2.506918	1.150547	0.035467
16	1	0	0.008252	-2.721158	-0.051511
17	1	0	-4.592712	-1.550643	0.033268
18	1	0	-2.430459	-2.749534	-0.026044
19	1	0	-2.553209	2.225956	0.066405
20	1	0	-4.626226	0.950882	0.090678
21	1	0	4.599910	-1.540954	0.030101
22	1	0	4.629115	0.961215	0.094352
23	1	0	2.560549	2.232814	0.073625
24	6	0	-0.022915	2.724563	-0.064037
25	1	0	-0.168231	3.150978	0.938903
26	1	0	0.901268	3.143022	-0.466260
27	1	0	-0.833105	3.098966	-0.696777

```
 Rotational constants (GHZ):      1.3936698      0.4479973
0.3398550
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9809640798 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
       Virtual  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860581260     A.U. after   11 cycles
             Convg  =    0.4076D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
```

1	6	-0.000107169	0.000053972	-0.000029499
2	6	0.000073850	-0.000052330	0.000010718
3	6	0.000173079	-0.000022595	0.000027823
4	6	-0.000050293	-0.000008616	0.000009782
5	6	-0.000042108	0.000084066	-0.000003392
6	6	-0.000058970	-0.000089228	0.000017024
7	6	-0.000022692	0.000012359	-0.000064800
8	6	-0.000200926	-0.000236743	0.000080823
9	6	0.000232439	-0.000061473	-0.000055527
10	6	0.000001121	-0.000181127	0.000039392
11	6	0.000039129	-0.000038326	0.000007106
12	1	-0.000089855	-0.000017657	0.000000124
13	6	-0.000051299	0.000102825	-0.000030422
14	6	0.000143343	-0.000022114	0.000019204
15	6	0.000065729	0.000289251	-0.000004856
16	1	-0.000021055	0.000025819	0.000049530
17	1	-0.000090698	0.000070020	0.000035200
18	1	0.000055523	0.000071074	-0.000011741
19	1	0.000063411	-0.000092369	-0.000046245
20	1	0.000016226	-0.000090668	-0.000027902
21	1	-0.000015877	0.000113125	0.000030399
22	1	0.000081111	-0.000062542	-0.000034239
23	1	0.000109706	-0.000193753	-0.000072456
24	6	-0.000308514	0.000268350	-0.000068224
25	1	-0.000010031	-0.000025510	-0.000037679
26	1	-0.000069864	0.000010694	0.000100718
27	1	0.000084684	0.000093497	0.000059140

Cartesian Forces: Max   0.000308514 RMS   0.000096567

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal Forces: Max   0.000571379 RMS   0.000092797
 Search for a local minimum.
 Step number 28 out of a maximum of 157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points   1   2   3   4
5
                                                      6   7   8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
21
                                                     20   23   22   25
24
                                                     27   26   28

This journal is © The Royal Society of Chemistry 2014

```
 DE= -3.04D-06 DEPred=-3.34D-05 R= 9.10D-02
 Trust test= 9.10D-02 RLast= 4.91D-02 DXMaxT set to 5.00D-02
 Use linear search instead of GDIIS.
 Linear search step of   0.098 exceeds DXMaxT=   0.050 but not scaled.
 Quartic linear search produced a step of  2.00000.
 Iteration  1 RMS(Cart)=  0.01183110 RMS(Int)=  0.00020902
 Iteration  2 RMS(Cart)=  0.00021683 RMS(Int)=  0.00000081
 Iteration  3 RMS(Cart)=  0.00000006 RMS(Int)=  0.00000081
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58983   0.00014   0.00039   0.00000   0.00039
2.59022
    R2        2.69216  -0.00014  -0.00040   0.00000  -0.00040
2.69177
    R3        2.05402  -0.00002   0.00016   0.00000   0.00016
2.05419
    R4        2.70464   0.00000  -0.00032   0.00000  -0.00032
2.70432
    R5        2.05601  -0.00003   0.00008   0.00000   0.00008
2.05608
    R6        2.73332   0.00007  -0.00078   0.00000  -0.00078
2.73254
    R7        2.64270  -0.00010   0.00018   0.00000   0.00018
2.64288
    R8        2.71162   0.00008  -0.00050   0.00000  -0.00050
2.71111
    R9        2.67935   0.00013   0.00013   0.00000   0.00013
2.67948
   R10        2.59497   0.00009   0.00024   0.00000   0.00025
2.59521
   R11        2.04940  -0.00011   0.00028   0.00000   0.00028
2.04968
   R12        2.05446  -0.00002   0.00014   0.00000   0.00014
2.05460
   R13        2.64172  -0.00009  -0.00022   0.00000  -0.00022
2.64149
   R14        2.05711  -0.00003   0.00009   0.00000   0.00009
2.05721
   R15        2.67776   0.00057  -0.00057   0.00000  -0.00057
2.67719
   R16        2.86081   0.00045   0.00021   0.00000   0.00021
2.86102
   R17        2.73737   0.00011   0.00049   0.00000   0.00049
2.73786
   R18        2.71296   0.00028  -0.00006   0.00000  -0.00006
2.71290
   R19        2.70554   0.00000   0.00001   0.00000   0.00001
2.70555
   R20        2.05598  -0.00003   0.00007   0.00000   0.00007
2.05605
```

This journal is © The Royal Society of Chemistry 2014

R21	2.58885	0.00009	0.00007	0.00000	0.00007
2.58892					
R22	2.69261	-0.00019	-0.00021	0.00000	-0.00021
2.69241					
R23	2.05399	-0.00002	0.00015	0.00000	0.00015
2.05413					
R24	2.59400	0.00010	-0.00008	0.00000	-0.00008
2.59392					
R25	2.05444	-0.00001	0.00013	0.00000	0.00013
2.05457					
R26	2.04897	-0.00022	0.00015	0.00000	0.00015
2.04912					
R27	2.07770	-0.00004	-0.00020	0.00000	-0.00020
2.07750					
R28	2.06232	-0.00007	-0.00089	0.00000	-0.00089
2.06143					
R29	2.06745	-0.00011	0.00066	0.00000	0.00066
2.06812					
A1	2.08973	0.00002	0.00045	0.00000	0.00045
2.09018					
A2	2.10135	0.00011	-0.00076	0.00000	-0.00076
2.10059					
A3	2.09210	-0.00012	0.00031	0.00000	0.00031
2.09241					
A4	2.11596	0.00001	-0.00011	0.00000	-0.00011
2.11585					
A5	2.10356	0.00008	-0.00049	0.00000	-0.00049
2.10307					
A6	2.06365	-0.00009	0.00061	0.00000	0.00061
2.06425					
A7	2.08473	-0.00001	-0.00058	0.00000	-0.00058
2.08415					
A8	2.11386	-0.00008	0.00108	0.00000	0.00108
2.11494					
A9	2.08460	0.00009	-0.00050	0.00000	-0.00050
2.08409					
A10	2.04527	-0.00004	0.00105	0.00000	0.00105
2.04632					
A11	2.09531	-0.00001	0.00061	0.00000	0.00061
2.09592					
A12	2.14257	0.00005	-0.00167	0.00000	-0.00167
2.14090					
A13	2.12357	0.00003	-0.00042	0.00000	-0.00042
2.12315					
A14	2.08676	-0.00002	-0.00042	0.00000	-0.00042
2.08634					
A15	2.07275	-0.00001	0.00083	0.00000	0.00083
2.07358					
A16	2.10695	-0.00001	-0.00041	0.00000	-0.00041
2.10654					
A17	2.08684	-0.00009	0.00054	0.00000	0.00054
2.08738					

This journal is © The Royal Society of Chemistry 2014

A18	2.08939	0.00010	-0.00013	0.00000	-0.00013
2.08926					
A19	2.11889	0.00006	-0.00006	0.00000	-0.00006
2.11883					
A20	2.08240	-0.00003	0.00011	0.00000	0.00011
2.08251					
A21	2.08185	-0.00003	-0.00006	0.00000	-0.00005
2.08180					
A22	2.08788	-0.00011	0.00000	0.00000	0.00000
2.08788					
A23	2.08629	-0.00006	-0.00351	0.00000	-0.00351
2.08278					
A24	2.10894	0.00017	0.00351	0.00000	0.00352
2.11246					
A25	2.09102	-0.00008	-0.00065	0.00000	-0.00065
2.09036					
A26	2.15028	0.00021	0.00066	0.00000	0.00067
2.15095					
A27	2.04184	-0.00013	-0.00002	0.00000	-0.00002
2.04182					
A28	2.08769	0.00005	0.00044	0.00000	0.00044
2.08813					
A29	2.10995	-0.00008	-0.00009	0.00000	-0.00009
2.10985					
A30	2.08554	0.00002	-0.00035	0.00000	-0.00035
2.08519					
A31	2.06265	-0.00011	0.00026	0.00000	0.00026
2.06291					
A32	2.11689	0.00003	0.00020	0.00000	0.00020
2.11708					
A33	2.10363	0.00007	-0.00046	0.00000	-0.00046
2.10317					
A34	2.08854	0.00004	0.00007	0.00000	0.00007
2.08861					
A35	2.10203	0.00010	-0.00052	0.00000	-0.00052
2.10151					
A36	2.09260	-0.00014	0.00046	0.00000	0.00046
2.09306					
A37	2.10787	0.00000	-0.00014	0.00000	-0.00014
2.10773					
A38	2.08690	-0.00010	0.00057	0.00000	0.00057
2.08746					
A39	2.08841	0.00011	-0.00043	0.00000	-0.00043
2.08798					
A40	2.12549	0.00004	0.00021	0.00000	0.00021
2.12570					
A41	2.08913	-0.00001	0.00029	0.00000	0.00029
2.08942					
A42	2.06844	-0.00003	-0.00051	0.00000	-0.00051
2.06793					
A43	1.95119	-0.00006	0.00098	0.00000	0.00098
1.95216					

A44	1.95881	0.00009	0.00193	0.00000	0.00193	1.96074
A45	1.94399	0.00011	-0.00289	0.00000	-0.00289	1.94110
A46	1.87488	-0.00005	0.00014	0.00000	0.00013	1.87501
A47	1.87231	-0.00004	-0.00085	0.00000	-0.00085	1.87146
A48	1.85745	-0.00006	0.00066	0.00000	0.00066	1.85811
D1	-0.00146	0.00000	-0.00059	0.00000	-0.00059	-0.00205
D2	3.13450	0.00001	-0.00067	0.00000	-0.00066	3.13383
D3	-3.13899	0.00000	-0.00030	0.00000	-0.00030	-3.13929
D4	-0.00303	0.00001	-0.00037	0.00000	-0.00037	-0.00341
D5	0.00985	-0.00001	0.00091	0.00000	0.00091	0.01076
D6	-3.12888	-0.00002	0.00141	0.00000	0.00141	-3.12747
D7	-3.13579	-0.00001	0.00062	0.00000	0.00062	-3.13517
D8	0.00867	-0.00002	0.00112	0.00000	0.00112	0.00979
D9	-0.01302	0.00001	-0.00070	0.00000	-0.00070	-0.01373
D10	3.12531	0.00001	-0.00091	0.00000	-0.00091	3.12440
D11	3.13408	0.00000	-0.00063	0.00000	-0.00063	3.13345
D12	-0.01078	0.00000	-0.00083	0.00000	-0.00083	-0.01161
D13	0.01875	-0.00002	0.00165	0.00000	0.00165	0.02040
D14	-3.13172	-0.00001	0.00018	0.00000	0.00018	-3.13155
D15	-3.11964	-0.00002	0.00185	0.00000	0.00185	-3.11779
D16	0.01307	-0.00002	0.00038	0.00000	0.00038	0.01345
D17	-3.12102	-0.00003	0.00219	0.00000	0.00219	-3.11884
D18	0.01060	-0.00002	0.00171	0.00000	0.00171	0.01231
D19	0.01731	-0.00003	0.00198	0.00000	0.00198	0.01929
D20	-3.13425	-0.00002	0.00150	0.00000	0.00150	-3.13275
D21	-0.01086	0.00001	-0.00137	0.00000	-0.00137	-0.01223

This journal is © The Royal Society of Chemistry 2014

D22	3.11515	0.00003	-0.00186	0.00000	-0.00186	3.11329
D23	3.13988	0.00000	0.00013	0.00000	0.00013	3.14001
D24	-0.01730	0.00003	-0.00035	0.00000	-0.00035	-0.01766
D25	-0.04419	0.00007	-0.00327	0.00000	-0.00327	-0.04746
D26	3.11028	0.00008	-0.00364	0.00000	-0.00364	3.10664
D27	3.08801	0.00007	-0.00481	0.00000	-0.00481	3.08319
D28	-0.04071	0.00008	-0.00518	0.00000	-0.00518	-0.04589
D29	-0.00337	0.00001	0.00011	0.00000	0.00010	-0.00326
D30	3.13535	0.00002	-0.00039	0.00000	-0.00039	3.13496
D31	-3.12950	-0.00001	0.00060	0.00000	0.00060	-3.12890
D32	0.00923	-0.00001	0.00010	0.00000	0.00010	0.00933
D33	-0.01605	0.00002	-0.00142	0.00000	-0.00142	-0.01747
D34	3.12142	0.00003	-0.00177	0.00000	-0.00177	3.11965
D35	3.13551	0.00002	-0.00094	0.00000	-0.00094	3.13457
D36	-0.01021	0.00002	-0.00130	0.00000	-0.00130	-0.01150
D37	0.04537	-0.00008	0.00380	0.00000	0.00380	0.04917
D38	-3.08625	-0.00009	0.00455	0.00000	0.00455	-3.08170
D39	-3.10927	-0.00009	0.00412	0.00000	0.00412	-3.10515
D40	0.04230	-0.00010	0.00487	0.00000	0.00487	0.04716
D41	1.42760	-0.00004	-0.04084	0.00000	-0.04084	1.38676
D42	-2.74750	-0.00008	-0.03860	0.00000	-0.03860	-2.78610
D43	-0.66683	-0.00002	-0.03844	0.00000	-0.03844	-0.70527
D44	-1.70095	-0.00003	-0.04118	0.00000	-0.04118	-1.74214
D45	0.40713	-0.00007	-0.03894	0.00000	-0.03894	0.36819
D46	2.48780	-0.00001	-0.03878	0.00000	-0.03878	2.44901
D47	-0.01562	0.00003	-0.00151	0.00000	-0.00151	-0.01714

```
   D48        3.13004   0.00002  -0.00116   0.00000  -0.00116
3.12887
   D49        3.11660   0.00004  -0.00221   0.00000  -0.00221
3.11439
   D50       -0.02092   0.00003  -0.00186   0.00000  -0.00186  -
0.02278
   D51       -3.13865  -0.00001   0.00078   0.00000   0.00078  -
3.13787
   D52        0.01984  -0.00004   0.00146   0.00000   0.00146
0.02129
   D53        0.01266  -0.00002   0.00151   0.00000   0.00151
0.01417
   D54       -3.11204  -0.00005   0.00218   0.00000   0.00218  -
3.10986
   D55        0.01249  -0.00002   0.00117   0.00000   0.00117
0.01366
   D56       -3.12327  -0.00003   0.00121   0.00000   0.00121  -
3.12206
   D57       -3.13323  -0.00001   0.00082   0.00000   0.00082  -
3.13241
   D58        0.01420  -0.00002   0.00086   0.00000   0.00086
0.01506
   D59        0.00181   0.00000   0.00058   0.00000   0.00058
0.00239
   D60        3.13871   0.00000   0.00036   0.00000   0.00036
3.13908
   D61       -3.13381  -0.00001   0.00062   0.00000   0.00062  -
3.13319
   D62        0.00309  -0.00001   0.00040   0.00000   0.00040
0.00350
   D63       -0.01063   0.00002  -0.00098   0.00000  -0.00098  -
0.01161
   D64        3.12754   0.00003  -0.00163   0.00000  -0.00163
3.12591
   D65        3.13562   0.00001  -0.00076   0.00000  -0.00076
3.13486
   D66       -0.00939   0.00002  -0.00141   0.00000  -0.00141  -
0.01080
   D67        0.00301  -0.00001  -0.00011   0.00000  -0.00011
0.00291
   D68        3.12791   0.00002  -0.00077   0.00000  -0.00077
3.12714
   D69       -3.13516  -0.00002   0.00054   0.00000   0.00054  -
3.13462
   D70       -0.01026   0.00001  -0.00012   0.00000  -0.00012  -
0.01038
         Item               Value     Threshold  Converged?
 Maximum Force            0.000571     0.000450     NO
 RMS     Force            0.000093     0.000300     YES
 Maximum Displacement     0.077588     0.001800     NO
 RMS     Displacement     0.011835     0.001200     NO
 Predicted change in Energy=-3.605791D-06
```

This journal is © The Royal Society of Chemistry 2014

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.793241	-5.424309	0.018594
2	6	0	-3.423331	-5.395091	-0.017006
3	6	0	-2.707790	-4.155855	-0.032439
4	6	0	-3.443431	-2.910980	-0.027361
5	6	0	-4.874917	-2.994180	0.019278
6	6	0	-5.526046	-4.203098	0.043368
7	6	0	-1.309619	-4.127276	-0.048202
8	6	0	-2.749190	-1.674951	-0.054806
9	6	0	-1.332746	-1.666544	-0.028743
10	6	0	-0.605693	-2.919702	-0.036166
11	6	0	0.825893	-2.903592	-0.025557
12	1	0	1.350851	-3.856471	-0.040214
13	6	0	1.524180	-1.725421	0.009138
14	6	0	0.818557	-0.488008	0.038286
15	6	0	-0.553688	-0.461634	0.018326
16	1	0	-0.757367	-5.065347	-0.060400
17	1	0	-5.322283	-6.373817	0.032080
18	1	0	-2.851420	-6.320613	-0.028936
19	1	0	-5.462749	-2.083201	0.051285
20	1	0	-6.612180	-4.229331	0.084931
21	1	0	2.611125	-1.730173	0.019123
22	1	0	1.373616	0.445904	0.080626
23	1	0	-1.053031	0.500178	0.055509
24	6	0	-3.536818	-0.382597	-0.095119
25	1	0	-3.916841	-0.103879	0.898111
26	1	0	-2.942075	0.454155	-0.464051
27	1	0	-4.401195	-0.466181	-0.761137

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370684	0.000000			
3	C	2.441451	1.431063	0.000000		
4	C	2.853230	2.484214	1.445997	0.000000	
5	C	2.431502	2.805850	2.459390	1.434660	0.000000
6	C	1.424421	2.417830	2.819671	2.451909	1.373328
7	C	3.717846	2.464976	1.398552	2.456209	3.741632
8	C	4.270974	3.780917	2.481351	1.417918	2.502912
9	C	5.108627	4.274663	2.843841	2.450227	3.783107
10	C	4.879715	3.750600	2.438627	2.837765	4.270233
11	C	6.158785	4.925804	3.749017	4.269330	5.701706
12	H	6.341249	5.016044	4.069676	4.886641	6.285481
13	C	7.320634	6.159954	4.880401	5.107254	6.523672

14	C	7.473937	6.486611	5.088539	4.903024	6.220684
15	C	6.527018	5.707460	4.276682	3.788403	5.008674
16	H	4.052576	2.686630	2.152234	3.443447	4.609805
17	H	1.087029	2.136898	3.429153	3.940160	3.409142
18	H	2.139225	1.088032	2.169520	3.460646	3.893843
19	H	3.407684	3.890052	3.448579	2.183815	1.084644
20	H	2.177364	3.396785	3.906845	3.433894	2.132602
21	H	8.274738	7.060282	5.846149	6.168802	7.592005
22	H	8.514304	7.558932	6.151979	5.872331	7.133169
23	H	7.006431	6.354350	4.942126	4.166158	5.178673
24	C	5.197152	5.014387	3.863766	2.531014	2.936658
25	H	5.463388	5.392394	4.329692	2.993398	3.169242
26	H	6.181918	5.886012	4.636094	3.430188	3.982524
27	H	5.034353	5.079774	4.124599	2.726313	2.687794

		6	7	8	9	10
6	C	0.000000				
7	C	4.218102	0.000000			
8	C	3.756606	2.843643	0.000000		
9	C	4.901333	2.460918	1.416709	0.000000	
10	C	5.085597	1.397817	2.478776	1.448815	0.000000
11	C	6.483872	2.461367	3.780428	2.487975	1.431716
12	H	6.886134	2.674229	4.644306	3.463756	2.169244
13	C	7.473001	3.715187	4.274147	2.857784	2.442278
14	C	7.352272	4.216739	3.761159	2.453884	2.819071
15	C	6.222823	3.743366	2.509525	1.435603	2.459222
16	H	4.847117	1.088627	3.932198	3.447307	2.151136
17	H	2.180291	4.599442	5.357957	6.170780	5.846520
18	H	3.412143	2.681091	4.646858	4.895582	4.075480
19	H	2.120856	4.629970	2.746147	4.151738	4.929337
20	H	1.087246	5.305214	4.633257	5.869687	6.148795
21	H	8.504675	4.595962	5.361109	3.944675	3.430154
22	H	8.319852	5.303802	4.638308	3.434937	3.906226
23	H	6.490671	4.635722	2.760491	2.186326	3.450230
24	C	4.309574	4.357205	1.513988	2.551638	3.877095
25	H	4.485947	4.886802	2.177091	3.158880	4.445833
26	H	5.350176	4.881327	2.176644	2.697554	4.126097
27	H	3.984603	4.844557	2.165444	3.375300	4.577246

		11	12	13	14	15
11	C	0.000000				
12	H	1.088015	0.000000			
13	C	1.369998	2.138657	0.000000		
14	C	2.416438	3.411164	1.424761	0.000000	
15	C	2.805054	3.893022	2.432032	1.372644	0.000000
16	H	2.679760	2.430302	4.045417	4.842035	4.608889
17	H	7.060160	7.132529	8.275396	8.506039	7.595630
18	H	5.019828	4.871468	6.345323	6.891482	6.293603
19	H	6.342394	7.041165	6.996210	6.480711	5.170053
20	H	7.556105	7.972738	8.513264	8.319587	7.134795
21	H	2.136811	2.472440	1.087001	2.180972	3.409580
22	H	3.395643	4.304132	2.177712	1.087233	2.131198
23	H	3.888775	4.976767	3.405504	2.116519	1.084347
24	C	5.039196	5.996676	5.237151	4.358692	2.986332

This journal is © The Royal Society of Chemistry 2014

25	H	5.584360	6.535364	5.746684	4.828131	3.494683
26	H	5.065997	6.098389	4.992184	3.909267	2.603027
27	H	5.814163	6.715641	6.106479	5.280660	3.925671

		16	17	18	19	20
16	H	0.000000				
17	H	4.749643	0.000000			
18	H	2.441668	2.472188	0.000000		
19	H	5.571919	4.292957	4.978064	0.000000	
20	H	5.915986	2.503088	4.304618	2.434789	0.000000
21	H	4.740933	9.192528	7.135394	8.081652	9.556123
22	H	5.910572	9.557511	7.978012	7.289246	9.253690
23	H	5.574578	8.091901	7.054397	5.110721	7.298853
24	C	5.445613	6.252902	5.977807	2.573460	4.928248
25	H	5.959629	6.483625	6.375132	2.650408	4.994544
26	H	5.949856	7.247947	6.789331	3.613522	5.975457
27	H	5.909386	6.031397	6.100187	2.098018	4.445850

		21	22	23	24	25
21	H	0.000000				
22	H	2.504100	0.000000			
23	H	4.289735	2.427384	0.000000		
24	C	6.294935	4.982937	2.640298	0.000000	
25	H	6.784673	5.381401	3.045696	1.099367	0.000000
26	H	5.986884	4.349935	1.959732	1.090864	1.765518
27	H	7.167922	5.906683	3.579240	1.094401	1.766059

		26	27
26	H	0.000000	
27	H	1.750517	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.656066	-0.998005	0.025445
2	6	0	-2.458084	-1.663016	-0.011650
3	6	0	-1.215509	-0.953216	-0.023150
4	6	0	-1.223530	0.492719	-0.012412
5	6	0	-2.501911	1.142094	0.035587
6	6	0	-3.673581	0.425985	0.055784
7	6	0	0.006542	-1.633099	-0.040444
8	6	0	-0.000956	1.210531	-0.035911
9	6	0	1.226672	0.503851	-0.011479
10	6	0	1.223103	-0.944900	-0.024583
11	6	0	2.467707	-1.652496	-0.015593
12	1	0	2.440920	-2.740016	-0.034537
13	6	0	3.664559	-0.986941	0.022820
14	6	0	3.678682	0.437326	0.057563

```
     15          6           0        2.506752    1.151748    0.039316
     16          1           0        0.010791   -2.721593   -0.056904
     17          1           0       -4.591543   -1.551543    0.035894
     18          1           0       -2.430532   -2.750579   -0.027818
     19          1           0       -2.550562    2.225041    0.071793
     20          1           0       -4.624959    0.950538    0.098521
     21          1           0        4.600974   -1.538866    0.031511
     22          1           0        4.628719    0.964064    0.102849
     23          1           0        2.560143    2.233985    0.080791
     24          6           0       -0.029910    2.723851   -0.070320
     25          1           0       -0.218601    3.152209    0.924422
     26          1           0        0.905820    3.148283   -0.436724
     27          1           0       -0.817998    3.089884   -0.735639
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3938507      0.4480385
0.3399106
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       879.0205877329 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860584048     A.U. after   11 cycles
             Convg  =    0.4436D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000005457   -0.000143802   -0.000042176
      2        6          -0.000006955   -0.000135707   -0.000024936
      3        6           0.000148493   -0.000021794    0.000022875
      4        6           0.000000589    0.000147617    0.000109691
      5        6          -0.000119892    0.000050882   -0.000105822
      6        6          -0.000131647    0.000075858    0.000035444
      7        6           0.000000069   -0.000086351   -0.000087804
      8        6          -0.000401310   -0.000224939    0.000315330
      9        6           0.000211481   -0.000050879   -0.000074420
     10        6           0.000050107   -0.000121926    0.000049604
     11        6           0.000144362   -0.000002110   -0.000025442
     12        1          -0.000136221   -0.000015772    0.000007173
     13        6           0.000043008   -0.000069370   -0.000050957
     14        6           0.000063928    0.000097164    0.000051673
     15        6           0.000122887    0.000414049   -0.000080018
```

```
     16        1          -0.000040222    0.000052457    0.000075173
     17        1          -0.000107710    0.000140008    0.000053547
     18        1           0.000076988    0.000114428   -0.000009946
     19        1           0.000098947   -0.000147915   -0.000105944
     20        1           0.000067448   -0.000137695   -0.000035492
     21        1          -0.000067553    0.000160201    0.000051505
     22        1           0.000100619   -0.000132821   -0.000049887
     23        1           0.000124825   -0.000267549   -0.000123956
     24        6          -0.000300990    0.000146074   -0.000070324
     25        1           0.000031815   -0.000066488    0.000020357
     26        1           0.000010134    0.000102538    0.000077572
     27        1           0.000022257    0.000123844    0.000017180
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000414049 RMS     0.000124754


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000697090 RMS     0.000115885
 Search for a local minimum.
 Step number  29 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
21
                                                     20   23   22   25
24
                                                     27   26   28   29
     Eigenvalues ---   -0.07512   0.00040   0.00873   0.01542
0.01791
     Eigenvalues ---    0.01809   0.01824   0.01854   0.01920
0.01976
     Eigenvalues ---    0.01982   0.02012   0.02060   0.02099
0.02115
     Eigenvalues ---    0.02142   0.02189   0.02196   0.02234
0.02260
     Eigenvalues ---    0.02356   0.02537   0.05081   0.06922
0.09456
     Eigenvalues ---    0.11194   0.12506   0.15772   0.15991
0.15999
     Eigenvalues ---    0.16000   0.16001   0.16004   0.16019
0.16103
```

```
     Eigenvalues ---    0.16325   0.18480   0.21511   0.22001
0.22509
     Eigenvalues ---    0.22695   0.23512   0.23697   0.24453
0.24991
     Eigenvalues ---    0.25714   0.28253   0.32379   0.32949
0.33586
     Eigenvalues ---    0.33612   0.33631   0.33643   0.33682
0.33683
     Eigenvalues ---    0.33760   0.34130   0.35799   0.36701
0.37300
     Eigenvalues ---    0.37520   0.37651   0.38487   0.39644
0.40234
     Eigenvalues ---    0.40528   0.41150   0.42172   0.45337
0.46493
     Eigenvalues ---    0.48595   0.49830   0.50908   0.51259
0.55491
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is  -7.51D-02 should be greater than     0.000000
Eigenvector:
                          D40       D28       D38       D27       D39
   1                    0.26729  -0.26477   0.25846  -0.25647
0.24146
                          R16       D37       D26       D25       D17
```

```
   1                  -0.23954   0.23263  -0.23148  -0.22318
0.12987
 Use linear search instead of GDIIS.
 RFO step:  Lambda=-2.20491640D-05 EMin= 7.51232626D-02
 Quartic linear search produced a step of  0.01982.
 Iteration  1 RMS(Cart)=  0.00473702 RMS(Int)=  0.00000915
 Iteration  2 RMS(Cart)=  0.00001108 RMS(Int)=  0.00000136
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000136
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.59022   0.00008   0.00001   0.00043   0.00044
2.59065
    R2        2.69177  -0.00004  -0.00001   0.00017   0.00016
2.69193
    R3        2.05419  -0.00007   0.00000  -0.00076  -0.00076
2.05343
    R4        2.70432   0.00005  -0.00001   0.00065   0.00065
2.70496
    R5        2.05608  -0.00006   0.00000  -0.00076  -0.00076
2.05532
    R6        2.73254   0.00015  -0.00002   0.00108   0.00107
2.73361
    R7        2.64288  -0.00009   0.00000  -0.00072  -0.00072
2.64216
    R8        2.71111   0.00012  -0.00001   0.00079   0.00078
2.71189
    R9        2.67948   0.00014   0.00000   0.00007   0.00007
2.67955
   R10        2.59521   0.00008   0.00000   0.00002   0.00003
2.59524
   R11        2.04968  -0.00018   0.00001  -0.00136  -0.00136
2.04832
   R12        2.05460  -0.00007   0.00000  -0.00073  -0.00073
2.05387
   R13        2.64149  -0.00005   0.00000  -0.00033  -0.00034
2.64115
   R14        2.05721  -0.00007   0.00000  -0.00078  -0.00078
2.05643
   R15        2.67719   0.00070  -0.00001   0.00365   0.00364
2.68083
   R16        2.86102   0.00038   0.00000   0.00334   0.00335
2.86437
   R17        2.73786   0.00016   0.00001   0.00104   0.00105
2.73892
   R18        2.71290   0.00036   0.00000   0.00236   0.00235
2.71525
   R19        2.70555   0.00003   0.00000   0.00047   0.00047
2.70602
   R20        2.05605  -0.00005   0.00000  -0.00073  -0.00073
2.05532
```

This journal is © The Royal Society of Chemistry 2014

R21	2.58892	0.00002	0.00000	0.00012	0.00013
2.58905					
R22	2.69241	-0.00010	0.00000	-0.00033	-0.00034
2.69207					
R23	2.05413	-0.00007	0.00000	-0.00075	-0.00075
2.05338					
R24	2.59392	0.00011	0.00000	0.00027	0.00027
2.59419					
R25	2.05457	-0.00006	0.00000	-0.00071	-0.00071
2.05386					
R26	2.04912	-0.00030	0.00000	-0.00227	-0.00227
2.04685					
R27	2.07750	-0.00001	0.00000	0.00020	0.00020
2.07770					
R28	2.06143	0.00006	-0.00002	0.00104	0.00102
2.06245					
R29	2.06812	-0.00004	0.00001	-0.00007	-0.00006
2.06806					
A1	2.09018	-0.00002	0.00001	-0.00033	-0.00032
2.08986					
A2	2.10059	0.00018	-0.00002	0.00321	0.00319
2.10378					
A3	2.09241	-0.00016	0.00001	-0.00288	-0.00288
2.08954					
A4	2.11585	0.00001	0.00000	-0.00014	-0.00014
2.11571					
A5	2.10307	0.00013	-0.00001	0.00261	0.00260
2.10567					
A6	2.06425	-0.00014	0.00001	-0.00247	-0.00246
2.06180					
A7	2.08415	0.00005	-0.00001	0.00057	0.00055
2.08470					
A8	2.11494	-0.00016	0.00002	-0.00139	-0.00136
2.11358					
A9	2.08409	0.00011	-0.00001	0.00082	0.00081
2.08490					
A10	2.04632	-0.00012	0.00002	-0.00093	-0.00091
2.04541					
A11	2.09592	-0.00001	0.00001	-0.00012	-0.00011
2.09580					
A12	2.14090	0.00013	-0.00003	0.00105	0.00102
2.14192					
A13	2.12315	0.00005	-0.00001	0.00029	0.00029
2.12344					
A14	2.08634	-0.00003	-0.00001	-0.00047	-0.00048
2.08586					
A15	2.07358	-0.00002	0.00002	0.00020	0.00021
2.07379					
A16	2.10654	0.00003	-0.00001	0.00054	0.00053
2.10707					
A17	2.08738	-0.00016	0.00001	-0.00264	-0.00263
2.08475					

This journal is © The Royal Society of Chemistry 2014

A18	2.08926	0.00013	0.00000	0.00210	0.00210
2.09137					
A19	2.11883	0.00007	0.00000	0.00019	0.00019
2.11901					
A20	2.08251	-0.00004	0.00000	-0.00017	-0.00017
2.08234					
A21	2.08180	-0.00003	0.00000	0.00001	0.00001
2.08181					
A22	2.08788	-0.00012	0.00000	-0.00060	-0.00060
2.08728					
A23	2.08278	0.00003	-0.00007	0.00085	0.00078
2.08356					
A24	2.11246	0.00009	0.00007	-0.00025	-0.00018
2.11228					
A25	2.09036	-0.00007	-0.00001	-0.00026	-0.00028
2.09008					
A26	2.15095	0.00027	0.00001	0.00153	0.00155
2.15250					
A27	2.04182	-0.00019	0.00000	-0.00125	-0.00125
2.04058					
A28	2.08813	0.00004	0.00001	0.00013	0.00014
2.08827					
A29	2.10985	-0.00012	0.00000	-0.00089	-0.00089
2.10896					
A30	2.08519	0.00008	-0.00001	0.00076	0.00075
2.08594					
A31	2.06291	-0.00014	0.00001	-0.00252	-0.00252
2.06040					
A32	2.11708	0.00003	0.00000	-0.00008	-0.00007
2.11701					
A33	2.10317	0.00012	-0.00001	0.00260	0.00259
2.10576					
A34	2.08861	0.00002	0.00000	0.00007	0.00007
2.08868					
A35	2.10151	0.00016	-0.00001	0.00303	0.00302
2.10452					
A36	2.09306	-0.00018	0.00001	-0.00309	-0.00308
2.08998					
A37	2.10773	0.00003	0.00000	0.00048	0.00048
2.10821					
A38	2.08746	-0.00017	0.00001	-0.00280	-0.00279
2.08467					
A39	2.08798	0.00014	-0.00001	0.00232	0.00231
2.09030					
A40	2.12570	0.00003	0.00000	0.00009	0.00009
2.12579					
A41	2.08942	-0.00003	0.00001	-0.00106	-0.00105
2.08837					
A42	2.06793	0.00000	-0.00001	0.00101	0.00100
2.06893					
A43	1.95216	-0.00018	0.00002	-0.00417	-0.00415
1.94801					

This journal is © The Royal Society of Chemistry 2014

A44	1.96074	0.00008	0.00004	0.00026	0.00029	1.96103
A45	1.94110	0.00020	-0.00006	0.00380	0.00374	1.94485
A46	1.87501	-0.00002	0.00000	-0.00152	-0.00152	1.87349
A47	1.87146	-0.00001	-0.00002	0.00067	0.00065	1.87212
A48	1.85811	-0.00007	0.00001	0.00107	0.00108	1.85918
D1	-0.00205	0.00002	-0.00001	0.00065	0.00064	-0.00141
D2	3.13383	0.00003	-0.00001	0.00091	0.00090	3.13473
D3	-3.13929	0.00001	-0.00001	0.00086	0.00085	-3.13844
D4	-0.00341	0.00002	-0.00001	0.00112	0.00111	-0.00229
D5	0.01076	-0.00003	0.00002	-0.00015	-0.00014	0.01062
D6	-3.12747	-0.00004	0.00003	0.00012	0.00014	-3.12733
D7	-3.13517	-0.00002	0.00001	-0.00034	-0.00033	-3.13550
D8	0.00979	-0.00003	0.00002	-0.00007	-0.00005	0.00973
D9	-0.01373	0.00002	-0.00001	-0.00059	-0.00060	-0.01432
D10	3.12440	0.00004	-0.00002	-0.00117	-0.00118	3.12322
D11	3.13345	0.00001	-0.00001	-0.00086	-0.00087	3.13258
D12	-0.01161	0.00003	-0.00002	-0.00144	-0.00146	-0.01306
D13	0.02040	-0.00006	0.00003	0.00002	0.00005	0.02046
D14	-3.13155	-0.00001	0.00000	-0.00091	-0.00091	-3.13246
D15	-3.11779	-0.00007	0.00004	0.00060	0.00063	-3.11715
D16	0.01345	-0.00003	0.00001	-0.00034	-0.00033	0.01312
D17	-3.11884	-0.00009	0.00004	-0.00067	-0.00063	-3.11947
D18	0.01231	-0.00004	0.00003	0.00206	0.00209	0.01440
D19	0.01929	-0.00007	0.00004	-0.00126	-0.00122	0.01807
D20	-3.13275	-0.00003	0.00003	0.00148	0.00151	-3.13124
D21	-0.01223	0.00005	-0.00003	0.00047	0.00044	-0.01179

This journal is © The Royal Society of Chemistry 2014

D22	3.11329	0.00008	-0.00004	0.00177	0.00173	3.11502
D23	3.14001	0.00000	0.00000	0.00144	0.00144	3.14145
D24	-0.01766	0.00003	-0.00001	0.00274	0.00273	-0.01492
D25	-0.04746	0.00014	-0.00006	0.00293	0.00286	-0.04460
D26	3.10664	0.00011	-0.00007	0.00313	0.00306	3.10970
D27	3.08319	0.00019	-0.00010	0.00193	0.00183	3.08503
D28	-0.04589	0.00016	-0.00010	0.00213	0.00203	-0.04386
D29	-0.00326	-0.00001	0.00000	-0.00041	-0.00041	-0.00368
D30	3.13496	0.00001	-0.00001	-0.00069	-0.00070	3.13426
D31	-3.12890	-0.00004	0.00001	-0.00170	-0.00169	-3.13059
D32	0.00933	-0.00002	0.00000	-0.00198	-0.00198	0.00735
D33	-0.01747	0.00006	-0.00003	0.00032	0.00029	-0.01718
D34	3.11965	0.00008	-0.00004	0.00100	0.00096	3.12061
D35	3.13457	0.00002	-0.00002	-0.00241	-0.00243	3.13214
D36	-0.01150	0.00004	-0.00003	-0.00173	-0.00176	-0.01326
D37	0.04917	-0.00015	0.00008	-0.00387	-0.00379	0.04538
D38	-3.08170	-0.00018	0.00009	-0.00615	-0.00606	-3.08776
D39	-3.10515	-0.00013	0.00008	-0.00407	-0.00399	-3.10914
D40	0.04716	-0.00016	0.00010	-0.00635	-0.00625	0.04091
D41	1.38676	0.00000	-0.00081	0.00482	0.00401	1.39077
D42	-2.78610	-0.00010	-0.00076	0.00004	-0.00072	-2.78682
D43	-0.70527	0.00000	-0.00076	0.00419	0.00344	-0.70184
D44	-1.74214	-0.00002	-0.00082	0.00503	0.00421	-1.73793
D45	0.36819	-0.00013	-0.00077	0.00025	-0.00052	0.36766
D46	2.44901	-0.00002	-0.00077	0.00440	0.00364	2.45265
D47	-0.01714	0.00005	-0.00003	0.00228	0.00225	-0.01489

```
   D48        3.12887   0.00003  -0.00002   0.00161   0.00159
3.13046
   D49        3.11439   0.00008  -0.00004   0.00443   0.00439
3.11878
   D50       -0.02278   0.00007  -0.00004   0.00377   0.00373  -
0.01906
   D51       -3.13787  -0.00002   0.00002  -0.00127  -0.00125  -
3.13912
   D52        0.02129  -0.00006   0.00003  -0.00411  -0.00408
0.01721
   D53        0.01417  -0.00005   0.00003  -0.00350  -0.00347
0.01070
   D54       -3.10986  -0.00009   0.00004  -0.00633  -0.00629  -
3.11614
   D55        0.01366  -0.00004   0.00002  -0.00168  -0.00166
0.01200
   D56       -3.12206  -0.00005   0.00002  -0.00217  -0.00214  -
3.12420
   D57       -3.13241  -0.00002   0.00002  -0.00100  -0.00099  -
3.13340
   D58        0.01506  -0.00003   0.00002  -0.00149  -0.00147
0.01359
   D59        0.00239  -0.00002   0.00001  -0.00123  -0.00122
0.00117
   D60        3.13908  -0.00001   0.00001   0.00004   0.00005
3.13913
   D61       -3.13319  -0.00003   0.00001  -0.00172  -0.00171  -
3.13489
   D62        0.00350  -0.00002   0.00001  -0.00044  -0.00043
0.00307
   D63       -0.01161   0.00003  -0.00002   0.00160   0.00158  -
0.01004
   D64        3.12591   0.00005  -0.00003   0.00183   0.00180
3.12771
   D65        3.13486   0.00002  -0.00002   0.00031   0.00029
3.13515
   D66       -0.01080   0.00004  -0.00003   0.00054   0.00052  -
0.01028
   D67        0.00291   0.00000   0.00000   0.00086   0.00086
0.00376
   D68        3.12714   0.00004  -0.00002   0.00364   0.00363
3.13077
   D69       -3.13462  -0.00001   0.00001   0.00063   0.00064  -
3.13397
   D70       -0.01038   0.00002   0.00000   0.00342   0.00342  -
0.00697
         Item               Value     Threshold  Converged?
 Maximum Force            0.000697     0.000450     NO
 RMS     Force            0.000116     0.000300     YES
 Maximum Displacement     0.023852     0.001800     NO
 RMS     Displacement     0.004736     0.001200     NO
 Predicted change in Energy=-2.415771D-05
```

This journal is © The Royal Society of Chemistry 2014

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.792222	-5.426263	0.016982
2	6	0	-3.422093	-5.395432	-0.017707
3	6	0	-2.707991	-4.154962	-0.032325
4	6	0	-3.444869	-2.910159	-0.028152
5	6	0	-4.876676	-2.995775	0.016890
6	6	0	-5.526145	-4.205603	0.040808
7	6	0	-1.310172	-4.126459	-0.045718
8	6	0	-2.751355	-1.673640	-0.053694
9	6	0	-1.332972	-1.665277	-0.028298
10	6	0	-0.606086	-2.919186	-0.033643
11	6	0	0.825757	-2.904653	-0.021791
12	1	0	1.347074	-3.859124	-0.033990
13	6	0	1.525286	-1.727071	0.010452
14	6	0	0.821121	-0.488919	0.034214
15	6	0	-0.551213	-0.460432	0.013369
16	1	0	-0.758333	-5.064286	-0.058652
17	1	0	-5.322977	-6.374349	0.030726
18	1	0	-2.846916	-6.318450	-0.029817
19	1	0	-5.465288	-2.086076	0.046544
20	1	0	-6.611819	-4.235611	0.081774
21	1	0	2.611831	-1.729656	0.021442
22	1	0	1.379616	0.442663	0.072901
23	1	0	-1.049394	0.500895	0.042887
24	6	0	-3.539685	-0.379549	-0.091019
25	1	0	-3.913656	-0.104279	0.905582
26	1	0	-2.944774	0.458558	-0.458198
27	1	0	-4.407478	-0.458918	-0.753048

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370915	0.000000			
3	C	2.441855	1.431405	0.000000		
4	C	2.854501	2.485399	1.446562	0.000000	
5	C	2.431955	2.806307	2.459539	1.435071	0.000000
6	C	1.424507	2.417881	2.819558	2.452477	1.373342
7	C	3.717270	2.463998	1.398173	2.456954	3.741966
8	C	4.272273	3.781920	2.481793	1.417954	2.503999
9	C	5.110135	4.275347	2.844156	2.451498	3.785512
10	C	4.879727	3.749925	2.438267	2.838802	4.271575
11	C	6.158061	4.924249	3.748434	4.270634	5.703292
12	H	6.336362	5.010535	4.065842	4.885006	6.283552
13	C	7.320859	6.159077	4.880279	5.109171	6.526467

14	C	7.475780	6.487020	5.089099	4.905605	6.224911
15	C	6.530364	5.709391	4.278239	3.791587	5.013741
16	H	4.050804	2.684577	2.151449	3.443642	4.609251
17	H	1.086626	2.138687	3.430423	3.940985	3.407952
18	H	2.140655	1.087629	2.167945	3.460346	3.893876
19	H	3.407453	3.889808	3.448071	2.183297	1.083926
20	H	2.175495	3.395501	3.906328	3.434891	2.133571
21	H	8.275562	7.060289	5.846837	6.170872	7.594789
22	H	8.516983	7.559627	6.152866	5.875992	7.139130
23	H	7.010038	6.356103	4.943036	4.168769	5.184155
24	C	5.200945	5.017796	3.866381	2.533166	2.940039
25	H	5.466717	5.393550	4.329125	2.994091	3.174575
26	H	6.186273	5.889912	4.639181	3.432680	3.986273
27	H	5.041377	5.087325	4.131396	2.731423	2.692321

		6	7	8	9	10
6	C	0.000000				
7	C	4.217603	0.000000			
8	C	3.757557	2.844889	0.000000		
9	C	4.903135	2.461350	1.418635	0.000000	
10	C	5.086000	1.397638	2.480718	1.449372	0.000000
11	C	6.484062	2.460809	3.783139	2.489218	1.431966
12	H	6.882353	2.670686	4.644765	3.463473	2.167561
13	C	7.474405	3.714841	4.277456	2.859189	2.442505
14	C	7.355377	4.216693	3.764820	2.455166	2.819170
15	C	6.227119	3.744231	2.513363	1.436849	2.459816
16	H	4.845541	1.088216	3.933019	3.447375	2.150641
17	H	2.178264	4.600158	5.358827	6.172437	5.847337
18	H	3.412825	2.677061	4.645854	4.893265	4.071404
19	H	2.120409	4.629974	2.746923	4.154360	4.930755
20	H	1.086861	5.304302	4.635217	5.872390	6.149400
21	H	8.506313	4.596878	5.364005	3.945642	3.431182
22	H	8.324479	5.303387	4.643241	3.436828	3.905943
23	H	6.495570	4.635544	2.763078	2.185815	3.449541
24	C	4.313015	4.360289	1.515760	2.554724	3.880599
25	H	4.490970	4.884775	2.175787	3.157337	4.443631
26	H	5.354147	4.885125	2.178831	2.700629	4.130238
27	H	3.989896	4.852265	2.169652	3.381294	4.584871

		11	12	13	14	15
11	C	0.000000				
12	H	1.087628	0.000000			
13	C	1.370065	2.139949	0.000000		
14	C	2.416387	3.411680	1.424582	0.000000	
15	C	2.805619	3.893179	2.432331	1.372788	0.000000
16	H	2.678566	2.426059	4.044341	4.841206	4.609074
17	H	7.060346	7.128823	8.276250	8.508127	7.598977
18	H	5.014240	4.861878	6.340231	6.887817	6.291939
19	H	6.344445	7.039777	6.999880	6.486139	5.176094
20	H	7.556435	7.968634	8.515300	8.323975	7.140560
21	H	2.138351	2.477361	1.086604	2.178586	3.408203
22	H	3.394149	4.303237	2.175515	1.086857	2.132423
23	H	3.888204	4.975815	3.404977	2.116279	1.083146
24	C	5.043612	5.999259	5.242141	4.363975	2.991388

This journal is © The Royal Society of Chemistry 2014

25	H	5.582486	6.531228	5.746025	4.829632	3.496986
26	H	5.071345	6.102646	4.997804	3.914352	2.606924
27	H	5.822637	6.722597	6.114641	5.287620	3.931689

		16	17	18	19	20
16	H	0.000000				
17	H	4.749761	0.000000			
18	H	2.436379	2.477431	0.000000		
19	H	5.571017	4.290663	4.977418	0.000000	
20	H	5.913520	2.497582	4.304086	2.436448	0.000000
21	H	4.741748	9.194261	7.131450	8.085018	9.558199
22	H	5.908859	9.560239	7.974131	7.297118	9.260095
23	H	5.573712	8.095223	7.052648	5.117866	7.305928
24	C	5.448278	6.255604	5.979483	2.576646	4.933263
25	H	5.957137	6.485779	6.374074	2.659516	5.002664
26	H	5.953316	7.251449	6.791239	3.617032	5.981138
27	H	5.916744	6.036949	6.106760	2.099036	4.451905

		21	22	23	24	25
21	H	0.000000				
22	H	2.497993	0.000000			
23	H	4.287236	2.429894	0.000000		
24	C	6.298936	4.990233	2.644742	0.000000	
25	H	6.782739	5.386208	3.051962	1.099473	0.000000
26	H	5.991177	4.356911	1.960955	1.091404	1.765053
27	H	7.175327	5.914854	3.582106	1.094370	1.766545

		26	27
26	H	0.000000	
27	H	1.751629	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.656057	-1.000402	0.023972
2	6	0	-2.457049	-1.664066	-0.012612
3	6	0	-1.215128	-0.952419	-0.023178
4	6	0	-1.224317	0.494076	-0.012794
5	6	0	-2.504214	1.141457	0.034010
6	6	0	-3.674875	0.423666	0.053906
7	6	0	0.006606	-1.632140	-0.038519
8	6	0	-0.002161	1.212733	-0.034270
9	6	0	1.227155	0.505088	-0.010934
10	6	0	1.223125	-0.944233	-0.022513
11	6	0	2.467188	-1.653273	-0.012717
12	1	0	2.436499	-2.740337	-0.029614
13	6	0	3.664793	-0.988803	0.023340
14	6	0	3.680493	0.435379	0.053239

```
     15          6           0        2.509517    1.151629    0.034538
     16          1           0        0.010669   -2.720205   -0.056127
     17          1           0       -4.592271   -1.551897    0.034597
     18          1           0       -2.425367   -2.751105   -0.029372
     19          1           0       -2.554227    2.223686    0.068278
     20          1           0       -4.627776    0.944669    0.096352
     21          1           0        4.601980   -1.538621    0.032715
     22          1           0        4.632309    0.958414    0.094935
     23          1           0        2.563630    2.232881    0.068749
     24          6           0       -0.030920    2.727906   -0.065103
     25          1           0       -0.216017    3.149835    0.933173
     26          1           0        0.905570    3.153598   -0.429707
     27          1           0       -0.819941    3.099502   -0.726171
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3922927      0.4478140
0.3396722
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.7627038950 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860585353     A.U. after   10 cycles
             Convg  =    0.9326D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000295898    0.000254386   -0.000021249
      2        6          -0.000249391    0.000294241   -0.000063974
      3        6          -0.000327093    0.000010327    0.000049522
      4        6           0.000046867   -0.000134026    0.000279144
      5        6           0.000253894   -0.000172907   -0.000185009
      6        6           0.000268044   -0.000048733    0.000043236
      7        6          -0.000089734    0.000126872   -0.000219684
      8        6           0.000456154    0.000380450   -0.000132074
      9        6          -0.000150277    0.000159870   -0.000223275
     10        6          -0.000010253    0.000451323    0.000073431
     11        6          -0.000222672    0.000220295   -0.000035016
     12        1           0.000236467   -0.000107026    0.000011458
     13        6          -0.000241545   -0.000082477   -0.000051322
     14        6          -0.000193935   -0.000219522    0.000062449
     15        6          -0.000214703   -0.000867738   -0.000121364
```

```
     16        1           0.000111516   -0.000188966    0.000177123
     17        1           0.000067382   -0.000265355    0.000024717
     18        1          -0.000020311   -0.000261170    0.000028739
     19        1          -0.000192389    0.000284809   -0.000026088
     20        1          -0.000204898    0.000141524   -0.000062250
     21        1           0.000204350   -0.000194216    0.000052785
     22        1          -0.000041405    0.000253613   -0.000088255
     23        1          -0.000202579    0.000521403    0.000042148
     24        6           0.000527596   -0.000233624    0.000451580
     25        1          -0.000125047    0.000014151   -0.000101054
     26        1          -0.000142749   -0.000239045    0.000053841
     27        1           0.000160812   -0.000098460   -0.000019560
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000867738 RMS     0.000226763


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000931268 RMS     0.000169250
 Search for a local minimum.
 Step number  30 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
21
                                                     20   23   22   25
24
                                                     27   26   28   29
30
 DE= -1.30D-06 DEPred=-2.42D-05 R= 5.40D-02
 Trust test= 5.40D-02 RLast= 2.41D-02 DXMaxT set to 5.00D-02
 Use linear search instead of GDIIS.
     Eigenvalues ---    0.00000   0.01284   0.01550   0.01788
0.01796
     Eigenvalues ---    0.01821   0.01866   0.01908   0.01971
0.01977
     Eigenvalues ---    0.01995   0.02068   0.02084   0.02114
0.02135
     Eigenvalues ---    0.02155   0.02201   0.02237   0.02245
0.02331
     Eigenvalues ---    0.02383   0.02570   0.06166   0.06983
0.12088
     Eigenvalues ---    0.12611   0.14509   0.15902   0.15999
0.16000
```

```
     Eigenvalues ---    0.16000   0.16002   0.16024   0.16054
0.16193
     Eigenvalues ---    0.16305   0.21046   0.21656   0.22016
0.22588
     Eigenvalues ---    0.22955   0.23767   0.24448   0.24881
0.24994
     Eigenvalues ---    0.25921   0.29656   0.32754   0.33567
0.33611
     Eigenvalues ---    0.33629   0.33632   0.33682   0.33686
0.33829
     Eigenvalues ---    0.34068   0.34237   0.36187   0.37035
0.37308
     Eigenvalues ---    0.37839   0.38164   0.39427   0.39770
0.40514
     Eigenvalues ---    0.40999   0.41776   0.42670   0.45309
0.48070
     Eigenvalues ---    0.48671   0.49839   0.51265   0.51410
0.55566
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-1.05747454D-04 EMin= 3.46637595D-06
 Quartic linear search produced a step of -0.46894.
 Maximum step size (   0.050) exceeded in Quadratic search.
    -- Step size scaled by   0.054
 Iteration  1 RMS(Cart)=  0.00639724 RMS(Int)=  0.00006135
```

This journal is © The Royal Society of Chemistry 2014

```
 Iteration  2 RMS(Cart)=  0.00006309 RMS(Int)=  0.00000044
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000044
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.59065  -0.00032  -0.00020   0.00002  -0.00018
2.59047
    R2        2.69193   0.00007  -0.00008   0.00004  -0.00004
2.69189
    R3        2.05343   0.00020   0.00036  -0.00001   0.00035
2.05378
    R4        2.70496  -0.00009  -0.00030   0.00000  -0.00030
2.70466
    R5        2.05532   0.00021   0.00036   0.00001   0.00036
2.05568
    R6        2.73361  -0.00025  -0.00050  -0.00037  -0.00087
2.73274
    R7        2.64216   0.00011   0.00034   0.00000   0.00034
2.64250
    R8        2.71189  -0.00019  -0.00036  -0.00002  -0.00039
2.71150
    R9        2.67955  -0.00020  -0.00003   0.00001  -0.00003
2.67952
   R10        2.59524  -0.00008  -0.00001  -0.00005  -0.00006
2.59518
   R11        2.04832   0.00034   0.00064   0.00000   0.00064
2.04896
   R12        2.05387   0.00020   0.00034   0.00004   0.00039
2.05425
   R13        2.64115   0.00018   0.00016  -0.00011   0.00005
2.64120
   R14        2.05643   0.00022   0.00036   0.00000   0.00037
2.05680
   R15        2.68083  -0.00093  -0.00171  -0.00010  -0.00180
2.67903
   R16        2.86437  -0.00070  -0.00157   0.00013  -0.00144
2.86293
   R17        2.73892  -0.00031  -0.00049   0.00022  -0.00028
2.73864
   R18        2.71525  -0.00066  -0.00110   0.00020  -0.00090
2.71435
   R19        2.70602  -0.00011  -0.00022   0.00012  -0.00011
2.70592
   R20        2.05532   0.00021   0.00034   0.00000   0.00034
2.05566
   R21        2.58905  -0.00021  -0.00006  -0.00012  -0.00018
2.58886
   R22        2.69207   0.00013   0.00016   0.00008   0.00024
2.69231
   R23        2.05338   0.00021   0.00035  -0.00001   0.00034
2.05372
```

This journal is © The Royal Society of Chemistry 2014

R24	2.59419	-0.00014	-0.00013	-0.00018	-0.00031
2.59388					
R25	2.05386	0.00019	0.00033	0.00004	0.00037
2.05424					
R26	2.04685	0.00056	0.00106	-0.00009	0.00098
2.04783					
R27	2.07770	-0.00004	-0.00009	0.00001	-0.00008
2.07762					
R28	2.06245	-0.00028	-0.00048	-0.00030	-0.00078
2.06167					
R29	2.06806	-0.00011	0.00003	0.00041	0.00044
2.06850					
A1	2.08986	0.00003	0.00015	0.00003	0.00018
2.09004					
A2	2.10378	-0.00021	-0.00150	0.00009	-0.00140
2.10237					
A3	2.08954	0.00018	0.00135	-0.00012	0.00123
2.09077					
A4	2.11571	-0.00002	0.00007	-0.00003	0.00004
2.11575					
A5	2.10567	-0.00015	-0.00122	0.00002	-0.00119
2.10447					
A6	2.06180	0.00017	0.00115	0.00000	0.00116
2.06295					
A7	2.08470	0.00000	-0.00026	-0.00004	-0.00029
2.08440					
A8	2.11358	0.00019	0.00064	0.00026	0.00090
2.11448					
A9	2.08490	-0.00019	-0.00038	-0.00022	-0.00060
2.08430					
A10	2.04541	0.00010	0.00043	0.00016	0.00059
2.04600					
A11	2.09580	0.00004	0.00005	0.00036	0.00041
2.09622					
A12	2.14192	-0.00014	-0.00048	-0.00052	-0.00100
2.14092					
A13	2.12344	-0.00008	-0.00013	-0.00005	-0.00019
2.12325					
A14	2.08586	0.00005	0.00023	-0.00021	0.00002
2.08588					
A15	2.07379	0.00003	-0.00010	0.00026	0.00016
2.07395					
A16	2.10707	-0.00003	-0.00025	-0.00007	-0.00032
2.10675					
A17	2.08475	0.00016	0.00123	-0.00009	0.00115
2.08589					
A18	2.09137	-0.00014	-0.00099	0.00016	-0.00083
2.09054					
A19	2.11901	-0.00008	-0.00009	-0.00002	-0.00010
2.11891					
A20	2.08234	0.00004	0.00008	0.00004	0.00013
2.08246					

This journal is © The Royal Society of Chemistry 2014

A21	2.08181	0.00004	0.00000	-0.00002	-0.00003
2.08178					
A22	2.08728	0.00022	0.00028	-0.00005	0.00023
2.08752					
A23	2.08356	-0.00011	-0.00036	-0.00165	-0.00202
2.08154					
A24	2.11228	-0.00011	0.00009	0.00171	0.00179
2.11407					
A25	2.09008	0.00006	0.00013	-0.00030	-0.00017
2.08992					
A26	2.15250	-0.00029	-0.00072	0.00066	-0.00006
2.15243					
A27	2.04058	0.00023	0.00059	-0.00036	0.00023
2.04080					
A28	2.08827	-0.00004	-0.00007	0.00023	0.00016
2.08843					
A29	2.10896	0.00007	0.00042	-0.00033	0.00009
2.10905					
A30	2.08594	-0.00004	-0.00035	0.00010	-0.00025
2.08569					
A31	2.06040	0.00019	0.00118	-0.00014	0.00104
2.06144					
A32	2.11701	-0.00006	0.00003	0.00011	0.00014
2.11715					
A33	2.10576	-0.00013	-0.00122	0.00003	-0.00118
2.10458					
A34	2.08868	-0.00005	-0.00003	-0.00015	-0.00018
2.08850					
A35	2.10452	-0.00017	-0.00142	0.00019	-0.00122
2.10330					
A36	2.08998	0.00022	0.00144	-0.00004	0.00140
2.09138					
A37	2.10821	-0.00002	-0.00022	0.00007	-0.00016
2.10805					
A38	2.08467	0.00018	0.00131	-0.00009	0.00122
2.08589					
A39	2.09030	-0.00016	-0.00108	0.00002	-0.00106
2.08923					
A40	2.12579	-0.00006	-0.00004	0.00023	0.00019
2.12598					
A41	2.08837	0.00009	0.00049	0.00016	0.00065
2.08902					
A42	2.06893	-0.00003	-0.00047	-0.00039	-0.00086
2.06807					
A43	1.94801	0.00022	0.00195	-0.00014	0.00180
1.94981					
A44	1.96103	-0.00002	-0.00014	0.00123	0.00109
1.96212					
A45	1.94485	-0.00026	-0.00176	-0.00091	-0.00266
1.94218					
A46	1.87349	0.00001	0.00071	0.00012	0.00083
1.87432					

This journal is © The Royal Society of Chemistry 2014

A47	1.87212	0.00000	-0.00031	-0.00023	-0.00054	1.87158
A48	1.85918	0.00005	-0.00050	-0.00009	-0.00059	1.85859
D1	-0.00141	0.00001	-0.00030	0.00008	-0.00021	-0.00163
D2	3.13473	0.00002	-0.00042	0.00009	-0.00033	3.13441
D3	-3.13844	-0.00001	-0.00040	-0.00003	-0.00043	-3.13887
D4	-0.00229	0.00000	-0.00052	-0.00002	-0.00055	-0.00284
D5	0.01062	-0.00003	0.00006	0.00002	0.00009	0.01071
D6	-3.12733	-0.00005	-0.00007	-0.00002	-0.00009	-3.12742
D7	-3.13550	-0.00001	0.00016	0.00014	0.00030	-3.13521
D8	0.00973	-0.00004	0.00002	0.00009	0.00012	0.00985
D9	-0.01432	0.00004	0.00028	0.00004	0.00032	-0.01400
D10	3.12322	0.00006	0.00056	0.00026	0.00081	3.12403
D11	3.13258	0.00003	0.00041	0.00003	0.00044	3.13302
D12	-0.01306	0.00004	0.00068	0.00025	0.00093	-0.01213
D13	0.02046	-0.00006	-0.00002	-0.00026	-0.00029	0.02017
D14	-3.13246	0.00000	0.00043	0.00008	0.00051	-3.13195
D15	-3.11715	-0.00008	-0.00030	-0.00048	-0.00077	-3.11793
D16	0.01312	-0.00002	0.00016	-0.00013	0.00003	0.01314
D17	-3.11947	-0.00008	0.00030	-0.00023	0.00006	-3.11941
D18	0.01440	-0.00010	-0.00098	0.00011	-0.00087	0.01353
D19	0.01807	-0.00007	0.00057	-0.00002	0.00055	0.01862
D20	-3.13124	-0.00008	-0.00071	0.00033	-0.00038	-3.13162
D21	-0.01179	0.00004	-0.00021	0.00038	0.00017	-0.01162
D22	3.11502	0.00006	-0.00081	0.00031	-0.00050	3.11453
D23	3.14145	-0.00002	-0.00068	0.00001	-0.00066	3.14079
D24	-0.01492	0.00000	-0.00128	-0.00005	-0.00133	-0.01626

This journal is © The Royal Society of Chemistry 2014

D25	-0.04460	0.00011	-0.00134	0.00016	-0.00118	-0.04578
D26	3.10970	0.00011	-0.00143	-0.00076	-0.00219	3.10751
D27	3.08503	0.00017	-0.00086	0.00053	-0.00033	3.08470
D28	-0.04386	0.00018	-0.00095	-0.00038	-0.00133	-0.04519
D29	-0.00368	0.00001	0.00019	-0.00026	-0.00007	-0.00375
D30	3.13426	0.00003	0.00033	-0.00022	0.00011	3.13437
D31	-3.13059	-0.00001	0.00079	-0.00020	0.00060	-3.12999
D32	0.00735	0.00001	0.00093	-0.00015	0.00078	0.00813
D33	-0.01718	0.00005	-0.00014	0.00013	-0.00001	-0.01718
D34	3.12061	0.00005	-0.00045	0.00024	-0.00021	3.12040
D35	3.13214	0.00007	0.00114	-0.00022	0.00092	3.13306
D36	-0.01326	0.00007	0.00083	-0.00011	0.00072	-0.01255
D37	0.04538	-0.00012	0.00178	-0.00006	0.00172	0.04709
D38	-3.08776	-0.00010	0.00284	-0.00019	0.00265	-3.08511
D39	-3.10914	-0.00012	0.00187	0.00084	0.00271	-3.10643
D40	0.04091	-0.00010	0.00293	0.00072	0.00365	0.04456
D41	1.39077	-0.00011	-0.00188	-0.02053	-0.02241	1.36837
D42	-2.78682	0.00005	0.00034	-0.01961	-0.01927	-2.80609
D43	-0.70184	-0.00009	-0.00161	-0.01952	-0.02113	-0.72297
D44	-1.73793	-0.00011	-0.00197	-0.02144	-0.02341	-1.76134
D45	0.36766	0.00005	0.00024	-0.02053	-0.02028	0.34738
D46	2.45265	-0.00009	-0.00170	-0.02043	-0.02214	2.43051
D47	-0.01489	0.00004	-0.00105	-0.00009	-0.00115	-0.01603
D48	3.13046	0.00004	-0.00074	-0.00020	-0.00094	3.12952
D49	3.11878	0.00002	-0.00206	0.00003	-0.00202	3.11676
D50	-0.01906	0.00002	-0.00175	-0.00008	-0.00182	-0.02088

```
   D51       -3.13912  -0.00002   0.00059   0.00004   0.00063  -
3.13850
   D52        0.01721  -0.00002   0.00191   0.00030   0.00221
0.01942
   D53        0.01070   0.00000   0.00163  -0.00008   0.00154
0.01224
   D54       -3.11614   0.00001   0.00295   0.00017   0.00312  -
3.11302
   D55        0.01200  -0.00002   0.00078  -0.00003   0.00075
0.01274
   D56       -3.12420  -0.00003   0.00101   0.00002   0.00103  -
3.12317
   D57       -3.13340  -0.00002   0.00046   0.00008   0.00054  -
3.13285
   D58        0.01359  -0.00002   0.00069   0.00013   0.00083
0.01442
   D59        0.00117   0.00000   0.00057  -0.00003   0.00055
0.00171
   D60        3.13913  -0.00001  -0.00002  -0.00003  -0.00005
3.13908
   D61       -3.13489  -0.00001   0.00080   0.00003   0.00083  -
3.13406
   D62        0.00307  -0.00001   0.00020   0.00003   0.00023
0.00330
   D63       -0.01004   0.00002  -0.00074  -0.00014  -0.00087  -
0.01091
   D64        3.12771   0.00004  -0.00084  -0.00016  -0.00101
3.12670
   D65        3.13515   0.00003  -0.00014  -0.00014  -0.00027
3.13488
   D66       -0.01028   0.00005  -0.00024  -0.00016  -0.00041  -
0.01069
   D67        0.00376  -0.00002  -0.00040   0.00019  -0.00021
0.00355
   D68        3.13077  -0.00002  -0.00170  -0.00006  -0.00176
3.12901
   D69       -3.13397  -0.00004  -0.00030   0.00022  -0.00008  -
3.13406
   D70       -0.00697  -0.00004  -0.00160  -0.00003  -0.00163  -
0.00860
         Item               Value     Threshold  Converged?
 Maximum Force            0.000931     0.000450     NO
 RMS     Force            0.000169     0.000300     YES
 Maximum Displacement     0.041098     0.001800     NO
 RMS     Displacement     0.006398     0.001200     NO
 Predicted change in Energy=-1.011635D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.792718	-5.424579	0.018880
2	6	0	-3.422677	-5.394869	-0.016447
3	6	0	-2.707608	-4.155148	-0.031601
4	6	0	-3.443554	-2.910330	-0.026881
5	6	0	-4.875232	-2.994293	0.018844
6	6	0	-5.525834	-4.203468	0.043115
7	6	0	-1.309629	-4.126582	-0.046632
8	6	0	-2.749899	-1.673929	-0.053560
9	6	0	-1.332467	-1.665392	-0.028423
10	6	0	-0.605688	-2.919188	-0.035005
11	6	0	0.826107	-2.904332	-0.024570
12	1	0	1.348712	-3.858288	-0.038182
13	6	0	1.525510	-1.726809	0.008424
14	6	0	0.820968	-0.488787	0.035098
15	6	0	-0.551228	-0.460849	0.015278
16	1	0	-0.757542	-5.064488	-0.059628
17	1	0	-5.323005	-6.373139	0.032589
18	1	0	-2.849254	-6.319203	-0.028538
19	1	0	-5.462968	-2.083655	0.049384
20	1	0	-6.611747	-4.231540	0.084506
21	1	0	2.612242	-1.730639	0.018340
22	1	0	1.378202	0.443715	0.075335
23	1	0	-1.049234	0.501022	0.048737
24	6	0	-3.540278	-0.382051	-0.093121
25	1	0	-3.935404	-0.116389	0.897862
26	1	0	-2.942421	0.461008	-0.442515
27	1	0	-4.394785	-0.459812	-0.772773

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370818	0.000000			
3	C	2.441656	1.431244	0.000000		
4	C	2.853731	2.484648	1.446102	0.000000	
5	C	2.431687	2.806052	2.459415	1.434866	0.000000
6	C	1.424485	2.417902	2.819630	2.452140	1.373309
7	C	3.717660	2.464637	1.398352	2.456277	3.741643
8	C	4.271502	3.781455	2.481677	1.417941	2.503126
9	C	5.109507	4.275292	2.844277	2.450829	3.784097
10	C	4.879662	3.750302	2.438376	2.837892	4.270544
11	C	6.158305	4.924937	3.748565	4.269667	5.702214
12	H	6.338271	5.012754	4.067174	4.885137	6.283885
13	C	7.320765	6.159532	4.880340	5.108186	6.525038
14	C	7.475010	6.486973	5.088959	4.904474	6.222902
15	C	6.529078	5.708833	4.277852	3.790420	5.011522
16	H	4.051971	2.685882	2.151847	3.443273	4.609472
17	H	1.086811	2.137911	3.429854	3.940421	3.408415
18	H	2.140013	1.087821	2.168688	3.460291	3.893824
19	H	3.407629	3.889891	3.448137	2.183401	1.084263

This journal is © The Royal Society of Chemistry 2014

20	H	2.176354	3.396129	3.906612	3.434450	2.133209
21	H	8.275181	7.060314	5.846499	6.169796	7.593358
22	H	8.515886	7.559492	6.152628	5.874470	7.136422
23	H	7.009087	6.356021	4.943337	4.168430	5.182313
24	C	5.196945	5.014783	3.864374	2.530995	2.935719
25	H	5.448346	5.381561	4.322379	2.983818	3.152503
26	H	6.186810	5.890966	4.640354	3.433629	3.985939
27	H	5.043211	5.086434	4.129335	2.732441	2.698347
		6	7	8	9	10
6	C	0.000000				
7	C	4.217861	0.000000			
8	C	3.756824	2.844281	0.000000		
9	C	4.902170	2.461364	1.417681	0.000000	
10	C	5.085598	1.397665	2.479648	1.449226	0.000000
11	C	6.483787	2.460843	3.781872	2.488862	1.431911
12	H	6.883686	2.671859	4.644381	3.463757	2.168317
13	C	7.473720	3.714828	4.276185	2.858874	2.442470
14	C	7.353966	4.216595	3.763444	2.454734	2.819062
15	C	6.225325	3.743875	2.512062	1.436373	2.459456
16	H	4.846495	1.088410	3.932609	3.447516	2.150809
17	H	2.179156	4.600052	5.358252	6.171790	5.847001
18	H	3.412558	2.679246	4.646404	4.894753	4.073541
19	H	2.120754	4.629578	2.745763	4.152353	4.929341
20	H	1.087064	5.304778	4.634038	5.871002	6.148926
21	H	8.505514	4.596285	5.362923	3.945526	3.430826
22	H	8.322443	5.303482	4.641363	3.436106	3.906035
23	H	6.494012	4.635905	2.762813	2.186212	3.449867
24	C	4.308622	4.358838	1.514996	2.554521	3.879724
25	H	4.468140	4.885531	2.176363	3.167443	4.451172
26	H	5.354176	4.885562	2.178602	2.699074	4.129421
27	H	3.994985	4.846718	2.167256	3.374207	4.577127
		11	12	13	14	15
11	C	0.000000				
12	H	1.087811	0.000000			
13	C	1.369968	2.139306	0.000000		
14	C	2.416287	3.411366	1.424707	0.000000	
15	C	2.805218	3.892970	2.432189	1.372623	0.000000
16	H	2.678703	2.427279	4.044386	4.841251	4.608868
17	H	7.060274	7.130308	8.275936	8.507291	7.597718
18	H	5.016935	4.866119	6.342713	6.889727	6.293104
19	H	6.342826	7.039600	6.997702	6.483183	5.172992
20	H	7.556127	7.970149	8.514365	8.322013	7.138123
21	H	2.137680	2.475196	1.086784	2.179711	3.408800
22	H	3.394732	4.303601	2.176546	1.087055	2.131794
23	H	3.888279	4.976071	3.405021	2.116026	1.083663
24	C	5.043007	5.999122	5.242222	4.364436	2.992053
25	H	5.594238	6.542161	5.762477	4.848311	3.514293
26	H	5.069714	6.101937	4.995228	3.910668	2.603306
27	H	5.813192	6.713942	6.104543	5.278028	3.923514
		16	17	18	19	20
16	H	0.000000				
17	H	4.750213	0.000000			

18	H	2.439372	2.475094	0.000000		
19	H	5.571201	4.291799	4.977695	0.000000	
20	H	5.914921	2.499999	4.304355	2.436050	0.000000
21	H	4.740894	9.193539	7.133376	8.082982	9.557241
22	H	5.909308	9.559158	7.976167	7.293139	9.257288
23	H	5.574202	8.094409	7.054184	5.114841	7.303422
24	C	5.447013	6.251964	5.977580	2.571478	4.927884
25	H	5.958127	6.466920	6.364970	2.631255	4.975825
26	H	5.954109	7.252480	6.793477	3.615305	5.980110
27	H	5.911104	6.039671	6.105327	2.110408	4.458226

		21	22	23	24	25
21	H	0.000000				
22	H	2.500783	0.000000			
23	H	4.288081	2.428259	0.000000		
24	C	6.299572	4.990162	2.646741	0.000000	
25	H	6.800811	5.405986	3.071186	1.099431	0.000000
26	H	5.989156	4.351581	1.956294	1.090989	1.765223
27	H	7.165144	5.904493	3.576421	1.094603	1.766349

		26	27
26	H	0.000000	
27	H	1.751097	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.655574	-0.999997	0.024548
2	6	0	-2.456956	-1.664162	-0.012099
3	6	0	-1.214827	-0.953205	-0.022877
4	6	0	-1.223724	0.492830	-0.012230
5	6	0	-2.502926	1.141124	0.034656
6	6	0	-3.673988	0.424052	0.054608
7	6	0	0.007328	-1.632512	-0.039262
8	6	0	-0.001753	1.211751	-0.034524
9	6	0	1.227074	0.505179	-0.010845
10	6	0	1.223531	-0.943988	-0.023381
11	6	0	2.467966	-1.652274	-0.014393
12	1	0	2.439045	-2.739550	-0.032503
13	6	0	3.665180	-0.987360	0.022736
14	6	0	3.679966	0.436899	0.055275
15	6	0	2.508584	1.152178	0.037016
16	1	0	0.011959	-2.720772	-0.056721
17	1	0	-4.591431	-1.552468	0.034892
18	1	0	-2.427058	-2.751447	-0.028619
19	1	0	-2.552109	2.223708	0.069582
20	1	0	-4.626323	0.946515	0.097027

This journal is © The Royal Society of Chemistry 2014

```
    21          1           0        4.602096   -1.538006    0.031491
    22          1           0        4.630953    0.961705    0.098782
    23          1           0        2.562719    2.233823    0.074980
    24          6           0       -0.033923    2.726037   -0.067906
    25          1           0       -0.242654    3.150471    0.924583
    26          1           0        0.907570    3.154714   -0.414439
    27          1           0       -0.810518    3.091993   -0.746973
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3930463      0.4479138
0.3397818
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8843496318 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860595349     A.U. after   10 cycles
             Convg  =    0.7690D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000131742    0.000091844   -0.000034921
      2        6          -0.000107983    0.000089868   -0.000037868
      3        6          -0.000117958   -0.000031539    0.000039161
      4        6          -0.000031765   -0.000016751    0.000186451
      5        6           0.000121368   -0.000015828   -0.000134508
      6        6           0.000059723   -0.000046624    0.000034635
      7        6          -0.000036654    0.000006720   -0.000171459
      8        6           0.000025555    0.000129287    0.000081574
      9        6           0.000065708    0.000094484   -0.000159553
     10        6           0.000049050    0.000178724    0.000061365
     11        6          -0.000059330    0.000094169   -0.000023101
     12        1           0.000064071   -0.000062128    0.000010072
     13        6          -0.000121421   -0.000044868   -0.000054085
     14        6          -0.000006259   -0.000084642    0.000052118
     15        6          -0.000136306   -0.000263904   -0.000092330
     16        1           0.000040314   -0.000075042    0.000137017
     17        1          -0.000004737   -0.000083380    0.000041034
     18        1           0.000021655   -0.000085951    0.000010652
     19        1          -0.000059601    0.000102643   -0.000077524
     20        1          -0.000061956    0.000021093   -0.000054414
     21        1           0.000078723   -0.000040575    0.000053039
```

This journal is © The Royal Society of Chemistry 2014

```
     22        1           0.000008360    0.000064497   -0.000074243
     23        1          -0.000080505    0.000165790   -0.000052189
     24        6           0.000138066   -0.000072084    0.000226658
     25        1          -0.000032168   -0.000024086   -0.000079215
     26        1          -0.000023748   -0.000073598    0.000096038
     27        1           0.000076056   -0.000018118    0.000015598
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000263904 RMS     0.000089706


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000249452 RMS     0.000068564
 Search for a local minimum.
 Step number  31 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8   10
9
                                                     11   12   13   14
15
                                                     16   17   18   19
21
                                                     20   23   22   25
24
                                                     27   26   28   29
30
                                                     31
 DE= -1.00D-05 DEPred=-1.01D-05 R= 9.88D-01
 SS=  1.41D+00  RLast= 5.39D-02 DXNew= 8.4090D-02 1.6180D-01
 Trust test= 9.88D-01 RLast= 5.39D-02 DXMaxT set to 8.41D-02
     Eigenvalues ---    0.00006   0.01487   0.01602   0.01707
0.01799
     Eigenvalues ---    0.01812   0.01852   0.01891   0.01970
0.01977
     Eigenvalues ---    0.02005   0.02049   0.02072   0.02109
0.02119
     Eigenvalues ---    0.02146   0.02195   0.02231   0.02252
0.02350
     Eigenvalues ---    0.02493   0.03937   0.06723   0.08356
0.10865
     Eigenvalues ---    0.13342   0.14983   0.15922   0.15998
0.16000
     Eigenvalues ---    0.16002   0.16003   0.16022   0.16078
0.16259
     Eigenvalues ---    0.16762   0.21256   0.22008   0.22151
0.22625
```

```
     Eigenvalues ---    0.23121   0.24417   0.24606   0.24864
0.25217
     Eigenvalues ---    0.28240   0.31705   0.32671   0.33367
0.33599
     Eigenvalues ---    0.33631   0.33681   0.33682   0.33717
0.33774
     Eigenvalues ---    0.34016   0.35027   0.35970   0.37220
0.37600
     Eigenvalues ---    0.37781   0.38194   0.39185   0.39787
0.40606
     Eigenvalues ---    0.41261   0.42526   0.43294   0.45449
0.48779
     Eigenvalues ---    0.49526   0.49948   0.51271   0.53845
0.73532
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   6.02D-05 Eigenvector:
                          D44       D46       D45       D41       D43
   1                    0.42715   0.41821   0.40725   0.40274
0.39380
                          D42       D28       D39       D26       A23
   1                    0.38284   0.03865  -0.03744   0.03452
0.03220
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    31   30
 RFO step:  Lambda=-2.03461837D-06.
```

This journal is © The Royal Society of Chemistry 2014

```
 DIIS coeffs:      1.42494     -0.42494
 Maximum step size (   0.084) exceeded in Quadratic search.
    -- Step size scaled by   0.117
 Iteration  1 RMS(Cart)=  0.00968764 RMS(Int)=  0.00015456
 Iteration  2 RMS(Cart)=  0.00016027 RMS(Int)=  0.00000056
 Iteration  3 RMS(Cart)=  0.00000003 RMS(Int)=  0.00000056
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59047  -0.00011  -0.00001  -0.00018  -0.00019
2.59028
    R2        2.69189   0.00002   0.00000   0.00084   0.00084
2.69273
    R3        2.05378   0.00008   0.00002  -0.00033  -0.00031
2.05346
    R4        2.70466  -0.00004  -0.00002   0.00029   0.00027
2.70493
    R5        2.05568   0.00008   0.00002  -0.00025  -0.00023
2.05545
    R6        2.73274  -0.00003  -0.00004  -0.00048  -0.00052
2.73221
    R7        2.64250   0.00006   0.00002   0.00041   0.00043
2.64293
    R8        2.71150  -0.00008  -0.00002   0.00023   0.00021
2.71172
    R9        2.67952  -0.00005   0.00000   0.00001   0.00001
2.67953
   R10        2.59518   0.00003   0.00000  -0.00032  -0.00032
2.59486
   R11        2.04896   0.00012   0.00003  -0.00010  -0.00007
2.04889
   R12        2.05425   0.00006   0.00002  -0.00030  -0.00028
2.05397
   R13        2.64120   0.00011   0.00000  -0.00006  -0.00006
2.64114
   R14        2.05680   0.00008   0.00002  -0.00026  -0.00024
2.05656
   R15        2.67903  -0.00020  -0.00009  -0.00082  -0.00091
2.67812
   R16        2.86293  -0.00025  -0.00007   0.00006  -0.00002
2.86291
   R17        2.73864  -0.00008  -0.00001   0.00065   0.00063
2.73927
   R18        2.71435  -0.00023  -0.00004   0.00058   0.00054
2.71489
   R19        2.70592  -0.00006  -0.00001   0.00063   0.00062
2.70654
   R20        2.05566   0.00008   0.00002  -0.00025  -0.00024
2.05543
   R21        2.58886  -0.00009  -0.00001  -0.00047  -0.00048
2.58838
```

This journal is © The Royal Society of Chemistry 2014

R22	2.69231	0.00003	0.00001	0.00106	0.00107
2.69338					
R23	2.05372	0.00008	0.00002	-0.00035	-0.00034
2.05339					
R24	2.59388	0.00002	-0.00002	-0.00061	-0.00063
2.59325					
R25	2.05424	0.00006	0.00002	-0.00030	-0.00028
2.05395					
R26	2.04783	0.00018	0.00005	-0.00014	-0.00010
2.04773					
R27	2.07762	-0.00006	0.00000	0.00029	0.00029
2.07791					
R28	2.06167	-0.00010	-0.00004	-0.00003	-0.00007
2.06160					
R29	2.06850	-0.00007	0.00002	0.00140	0.00143
2.06993					
A1	2.09004	0.00002	0.00001	-0.00021	-0.00020
2.08984					
A2	2.10237	-0.00005	-0.00007	0.00064	0.00057
2.10295					
A3	2.09077	0.00003	0.00006	-0.00043	-0.00037
2.09039					
A4	2.11575	-0.00001	0.00000	-0.00025	-0.00025
2.11550					
A5	2.10447	-0.00002	-0.00006	0.00034	0.00028
2.10475					
A6	2.06295	0.00003	0.00006	-0.00009	-0.00003
2.06292					
A7	2.08440	0.00002	-0.00001	0.00044	0.00043
2.08483					
A8	2.11448	0.00003	0.00004	-0.00006	-0.00002
2.11446					
A9	2.08430	-0.00005	-0.00003	-0.00038	-0.00041
2.08389					
A10	2.04600	0.00002	0.00003	-0.00007	-0.00004
2.04596					
A11	2.09622	0.00000	0.00002	0.00050	0.00053
2.09674					
A12	2.14092	-0.00003	-0.00005	-0.00043	-0.00048
2.14043					
A13	2.12325	-0.00004	-0.00001	-0.00015	-0.00016
2.12309					
A14	2.08588	0.00001	0.00000	-0.00037	-0.00037
2.08551					
A15	2.07395	0.00003	0.00001	0.00052	0.00052
2.07447					
A16	2.10675	0.00000	-0.00002	0.00023	0.00022
2.10697					
A17	2.08589	0.00002	0.00006	-0.00081	-0.00075
2.08514					
A18	2.09054	-0.00002	-0.00004	0.00058	0.00054
2.09107					

This journal is © The Royal Society of Chemistry 2014

A19	2.11891	-0.00001	-0.00001	-0.00018	-0.00018
2.11873					
A20	2.08246	0.00000	0.00001	0.00022	0.00023
2.08269					
A21	2.08178	0.00001	0.00000	-0.00005	-0.00005
2.08173					
A22	2.08752	0.00008	0.00001	0.00009	0.00010
2.08761					
A23	2.08154	0.00000	-0.00010	-0.00261	-0.00271
2.07883					
A24	2.11407	-0.00008	0.00009	0.00254	0.00263
2.11670					
A25	2.08992	0.00001	-0.00001	-0.00038	-0.00039
2.08953					
A26	2.15243	-0.00009	0.00000	0.00116	0.00116
2.15359					
A27	2.04080	0.00008	0.00001	-0.00078	-0.00077
2.04004					
A28	2.08843	-0.00001	0.00001	0.00030	0.00031
2.08874					
A29	2.10905	0.00001	0.00000	-0.00081	-0.00080
2.10825					
A30	2.08569	0.00001	-0.00001	0.00051	0.00050
2.08619					
A31	2.06144	0.00004	0.00005	-0.00040	-0.00035
2.06108					
A32	2.11715	-0.00003	0.00001	-0.00001	0.00000
2.11715					
A33	2.10458	-0.00001	-0.00006	0.00041	0.00035
2.10494					
A34	2.08850	0.00000	-0.00001	-0.00044	-0.00045
2.08805					
A35	2.10330	-0.00004	-0.00006	0.00079	0.00073
2.10403					
A36	2.09138	0.00004	0.00007	-0.00034	-0.00027
2.09110					
A37	2.10805	0.00000	-0.00001	0.00046	0.00046
2.10851					
A38	2.08589	0.00003	0.00006	-0.00072	-0.00066
2.08524					
A39	2.08923	-0.00003	-0.00005	0.00026	0.00020
2.08944					
A40	2.12598	-0.00005	0.00001	0.00026	0.00027
2.12625					
A41	2.08902	0.00003	0.00003	-0.00012	-0.00009
2.08893					
A42	2.06807	0.00002	-0.00004	-0.00015	-0.00019
2.06788					
A43	1.94981	0.00004	0.00009	-0.00147	-0.00138
1.94843					
A44	1.96212	-0.00001	0.00005	0.00123	0.00128
1.96341					

A45	1.94218	-0.00005	-0.00013	-0.00208	-0.00222	1.93996
A46	1.87432	-0.00001	0.00004	0.00140	0.00144	1.87576
A47	1.87158	-0.00001	-0.00003	0.00146	0.00143	1.87301
A48	1.85859	0.00004	-0.00003	-0.00035	-0.00038	1.85821
D1	-0.00163	0.00001	-0.00001	0.00019	0.00018	-0.00145
D2	3.13441	0.00003	-0.00002	-0.00022	-0.00024	3.13417
D3	-3.13887	0.00000	-0.00002	0.00052	0.00049	-3.13838
D4	-0.00284	0.00001	-0.00003	0.00010	0.00007	-0.00277
D5	0.01071	-0.00004	0.00000	0.00056	0.00057	0.01127
D6	-3.12742	-0.00005	0.00000	0.00026	0.00026	-3.12716
D7	-3.13521	-0.00002	0.00001	0.00024	0.00026	-3.13495
D8	0.00985	-0.00004	0.00001	-0.00005	-0.00005	0.00981
D9	-0.01400	0.00004	0.00002	-0.00066	-0.00064	-0.01464
D10	3.12403	0.00005	0.00004	-0.00032	-0.00028	3.12375
D11	3.13302	0.00002	0.00002	-0.00025	-0.00023	3.13279
D12	-0.01213	0.00004	0.00005	0.00008	0.00013	-0.01200
D13	0.02017	-0.00007	-0.00001	0.00038	0.00037	0.02054
D14	-3.13195	-0.00001	0.00003	0.00012	0.00015	-3.13180
D15	-3.11793	-0.00008	-0.00004	0.00005	0.00001	-3.11791
D16	0.01314	-0.00003	0.00000	-0.00021	-0.00021	0.01294
D17	-3.11941	-0.00009	0.00000	0.00050	0.00050	-3.11890
D18	0.01353	-0.00008	-0.00004	0.00057	0.00053	0.01406
D19	0.01862	-0.00007	0.00003	0.00084	0.00087	0.01949
D20	-3.13162	-0.00006	-0.00002	0.00091	0.00089	-3.13073
D21	-0.01162	0.00005	0.00001	0.00036	0.00037	-0.01125
D22	3.11453	0.00008	-0.00002	-0.00048	-0.00051	3.11402

D23	3.14079	-0.00001	-0.00003	0.00063	0.00059	3.14138
D24	-0.01626	0.00002	-0.00007	-0.00022	-0.00028	-0.01654
D25	-0.04578	0.00014	-0.00006	-0.00063	-0.00069	-0.04647
D26	3.10751	0.00013	-0.00011	-0.00272	-0.00283	3.10469
D27	3.08470	0.00019	-0.00002	-0.00091	-0.00093	3.08377
D28	-0.04519	0.00019	-0.00007	-0.00300	-0.00306	-0.04825
D29	-0.00375	0.00000	0.00000	-0.00084	-0.00085	-0.00459
D30	3.13437	0.00002	0.00001	-0.00055	-0.00054	3.13383
D31	-3.12999	-0.00003	0.00003	0.00000	0.00003	-3.12996
D32	0.00813	-0.00001	0.00004	0.00030	0.00034	0.00847
D33	-0.01718	0.00006	0.00000	-0.00063	-0.00063	-0.01781
D34	3.12040	0.00007	-0.00001	-0.00015	-0.00016	3.12024
D35	3.13306	0.00005	0.00005	-0.00070	-0.00065	3.13240
D36	-0.01255	0.00006	0.00004	-0.00022	-0.00018	-0.01273
D37	0.04709	-0.00015	0.00009	0.00083	0.00091	0.04800
D38	-3.08511	-0.00016	0.00013	0.00008	0.00021	-3.08490
D39	-3.10643	-0.00014	0.00014	0.00292	0.00306	-3.10337
D40	0.04456	-0.00015	0.00018	0.00217	0.00236	0.04692
D41	1.36837	-0.00005	-0.00112	-0.03270	-0.03382	1.33455
D42	-2.80609	-0.00005	-0.00096	-0.03108	-0.03204	-2.83813
D43	-0.72297	-0.00004	-0.00105	-0.03213	-0.03319	-0.75615
D44	-1.76134	-0.00006	-0.00117	-0.03480	-0.03597	-1.79731
D45	0.34738	-0.00005	-0.00101	-0.03318	-0.03419	0.31319
D46	2.43051	-0.00005	-0.00110	-0.03424	-0.03534	2.39517
D47	-0.01603	0.00005	-0.00006	-0.00022	-0.00028	-0.01631
D48	3.12952	0.00004	-0.00005	-0.00069	-0.00074	3.12878

```
   D49        3.11676   0.00006  -0.00010   0.00049   0.00039
3.11715
   D50       -0.02088   0.00005  -0.00009   0.00002  -0.00007  -
0.02095
   D51       -3.13850  -0.00002   0.00003   0.00001   0.00005  -
3.13845
   D52        0.01942  -0.00005   0.00011   0.00082   0.00093
0.02035
   D53        0.01224  -0.00002   0.00008  -0.00071  -0.00064
0.01161
   D54       -3.11302  -0.00005   0.00016   0.00009   0.00025  -
3.11277
   D55        0.01274  -0.00003   0.00004  -0.00040  -0.00036
0.01239
   D56       -3.12317  -0.00004   0.00005  -0.00003   0.00002  -
3.12315
   D57       -3.13285  -0.00002   0.00003   0.00008   0.00011  -
3.13274
   D58        0.01442  -0.00003   0.00004   0.00045   0.00049
0.01491
   D59        0.00171  -0.00001   0.00003  -0.00024  -0.00021
0.00150
   D60        3.13908   0.00000   0.00000  -0.00034  -0.00035
3.13873
   D61       -3.13406  -0.00002   0.00004   0.00014   0.00018  -
3.13388
   D62        0.00330  -0.00002   0.00001   0.00003   0.00004
0.00335
   D63       -0.01091   0.00003  -0.00004  -0.00046  -0.00050  -
0.01142
   D64        3.12670   0.00005  -0.00005  -0.00018  -0.00023
3.12648
   D65        3.13488   0.00003  -0.00001  -0.00036  -0.00037
3.13451
   D66       -0.01069   0.00005  -0.00002  -0.00007  -0.00009  -
0.01078
   D67        0.00355  -0.00001  -0.00001   0.00095   0.00094
0.00449
   D68        3.12901   0.00001  -0.00009   0.00015   0.00006
3.12907
   D69       -3.13406  -0.00003   0.00000   0.00066   0.00066  -
3.13340
   D70       -0.00860  -0.00001  -0.00008  -0.00013  -0.00021  -
0.00881
         Item               Value     Threshold  Converged?
 Maximum Force            0.000249     0.000450     YES
 RMS     Force            0.000069     0.000300     YES
 Maximum Displacement     0.062778     0.001800     NO
 RMS     Displacement     0.009690     0.001200     NO
 Predicted change in Energy=-6.210339D-06
```

This journal is © The Royal Society of Chemistry 2014

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.792581	-5.423671	0.021244
2	6	0	-3.422678	-5.394342	-0.015790
3	6	0	-2.707504	-4.154520	-0.031201
4	6	0	-3.442730	-2.909601	-0.025728
5	6	0	-4.874508	-2.992972	0.021458
6	6	0	-5.525300	-4.201830	0.046806
7	6	0	-1.309311	-4.126022	-0.047640
8	6	0	-2.749173	-1.673147	-0.052822
9	6	0	-1.332219	-1.664359	-0.028020
10	6	0	-0.605519	-2.918583	-0.035665
11	6	0	0.826624	-2.904715	-0.026487
12	1	0	1.348163	-3.859097	-0.040996
13	6	0	1.526729	-1.727915	0.006858
14	6	0	0.822213	-0.489253	0.034926
15	6	0	-0.549635	-0.460345	0.015511
16	1	0	-0.757145	-5.063715	-0.062050
17	1	0	-5.323576	-6.371636	0.035610
18	1	0	-2.849336	-6.318573	-0.028687
19	1	0	-5.461458	-2.081906	0.053070
20	1	0	-6.610995	-4.230200	0.089795
21	1	0	2.613289	-1.731709	0.016147
22	1	0	1.380226	0.442587	0.075656
23	1	0	-1.046751	0.501893	0.049993
24	6	0	-3.543127	-0.383565	-0.095268
25	1	0	-3.968625	-0.136854	0.888179
26	1	0	-2.939888	0.467693	-0.414068
27	1	0	-4.376612	-0.455654	-0.802315

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370717	0.000000			
3	C	2.441525	1.431388	0.000000		
4	C	2.853919	2.484842	1.445825	0.000000	
5	C	2.432079	2.806381	2.459243	1.434979	0.000000
6	C	1.424930	2.418062	2.819273	2.451982	1.373139
7	C	3.717770	2.464949	1.398580	2.455939	3.741552
8	C	4.271702	3.781835	2.481817	1.417948	2.502900
9	C	5.109693	4.275856	2.844700	2.450488	3.783580
10	C	4.879569	3.750489	2.438422	2.837243	4.270020
11	C	6.158156	4.924929	3.748612	4.269357	5.702017
12	H	6.337232	5.011840	4.066424	4.884101	6.282970
13	C	7.320690	6.159532	4.880429	5.108128	6.525061

14	C	7.474930	6.487031	5.088954	4.904234	6.222655
15	C	6.529719	5.709613	4.278493	3.790851	5.011862
16	H	4.052314	2.686358	2.152088	3.442948	4.609515
17	H	1.086645	2.138026	3.429854	3.940435	3.408406
18	H	2.139987	1.087699	2.168697	3.460233	3.894028
19	H	3.408197	3.890193	3.447766	2.183242	1.084228
20	H	2.176167	3.395842	3.906099	3.434418	2.133258
21	H	8.275114	7.060368	5.846630	6.169648	7.593281
22	H	8.515838	7.559497	6.152588	5.874381	7.136365
23	H	7.010305	6.357275	4.944378	4.169501	5.183302
24	C	5.193975	5.012855	3.862962	2.528987	2.931758
25	H	5.420416	5.362499	4.310142	2.966465	3.119173
26	H	6.191134	5.895352	4.643861	3.436536	3.988565
27	H	5.052967	5.091096	4.130635	2.738079	2.713759

		6	7	8	9	10
6	C	0.000000				
7	C	4.217728	0.000000			
8	C	3.756467	2.844262	0.000000		
9	C	4.901662	2.461847	1.417198	0.000000	
10	C	5.085054	1.397632	2.479245	1.449561	0.000000
11	C	6.483427	2.460540	3.782033	2.489796	1.432239
12	H	6.882563	2.670854	4.643994	3.464317	2.168287
13	C	7.473484	3.714433	4.276669	2.859867	2.442535
14	C	7.353523	4.216195	3.763523	2.454876	2.818695
15	C	6.225506	3.744099	2.512672	1.436656	2.459405
16	H	4.846648	1.088284	3.932456	3.447823	2.150646
17	H	2.179191	4.600438	5.358280	6.171987	5.847112
18	H	3.412782	2.679425	4.646569	4.895238	4.073659
19	H	2.120895	4.629133	2.744956	4.151088	4.928290
20	H	1.086916	5.304488	4.633846	5.870511	6.148319
21	H	8.505238	4.596041	5.363225	3.946330	3.431046
22	H	8.322123	5.302923	4.641634	3.436179	3.905513
23	H	6.494800	4.636385	2.763984	2.186373	3.449881
24	C	4.304456	4.358691	1.514987	2.555987	3.880645
25	H	4.433416	4.884789	2.175486	3.181717	4.461164
26	H	5.357351	4.888279	2.179465	2.698014	4.130294
27	H	4.009280	4.842465	2.166238	3.365833	4.568907

		11	12	13	14	15
11	C	0.000000				
12	H	1.087686	0.000000			
13	C	1.369714	2.139186	0.000000		
14	C	2.416246	3.411486	1.425276	0.000000	
15	C	2.805494	3.893116	2.432713	1.372291	0.000000
16	H	2.677848	2.425669	4.043314	4.840400	4.608697
17	H	7.060337	7.129574	8.275968	8.507241	7.598307
18	H	5.016684	4.864995	6.342346	6.889506	6.293601
19	H	6.342185	7.038337	6.997299	6.482391	5.172704
20	H	7.555701	7.968879	8.514157	8.321676	7.138446
21	H	2.137740	2.475801	1.086606	2.179908	3.408879
22	H	3.394309	4.303385	2.176528	1.086905	2.131494
23	H	3.888491	4.976156	3.405393	2.115568	1.083612
24	C	5.045359	6.000583	5.246060	4.368560	2.996525

This journal is © The Royal Society of Chemistry 2014

25	H	5.611780	6.556424	5.788532	4.878970	3.543400
26	H	5.070499	6.103088	4.994851	3.907780	2.599827
27	H	5.802885	6.703439	6.092852	5.265918	3.913389

		16	17	18	19	20
16	H	0.000000				
17	H	4.751050	0.000000			
18	H	2.439886	2.475643	0.000000		
19	H	5.570906	4.291981	4.977872	0.000000	
20	H	5.914842	2.499226	4.304116	2.436792	0.000000
21	H	4.740064	9.193645	7.133134	8.082421	9.556950
22	H	5.908187	9.559089	7.975799	7.292613	9.257146
23	H	5.574264	8.095482	7.055088	5.115238	7.304458
24	C	5.446705	6.248529	5.975793	2.566390	4.923684
25	H	5.957389	6.437023	6.348787	2.590209	4.937106
26	H	5.956908	7.256762	6.797803	3.616212	5.983403
27	H	5.906162	6.049603	6.107773	2.133839	4.476106

		21	22	23	24	25
21	H	0.000000				
22	H	2.500310	0.000000			
23	H	4.287892	2.427837	0.000000		
24	C	6.303282	4.995112	2.652740	0.000000	
25	H	6.828293	5.441153	3.106106	1.099582	0.000000
26	H	5.988341	4.347855	1.949484	1.090950	1.766246
27	H	7.152406	5.892270	3.568094	1.095358	1.768009

		26	27
26	H	0.000000	
27	H	1.751423	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.654835	-1.001427	0.024911
2	6	0	-2.456137	-1.665182	-0.012767
3	6	0	-1.214255	-0.953501	-0.023237
4	6	0	-1.223289	0.492252	-0.011984
5	6	0	-2.502667	1.140396	0.035649
6	6	0	-3.673347	0.423041	0.056152
7	6	0	0.008438	-1.632291	-0.040340
8	6	0	-0.001763	1.211946	-0.034139
9	6	0	1.227156	0.506518	-0.010096
10	6	0	1.224144	-0.942978	-0.023556
11	6	0	2.468773	-1.651594	-0.015125
12	1	0	2.439331	-2.738717	-0.034041
13	6	0	3.665841	-0.986990	0.022898
14	6	0	3.680161	0.437813	0.056702

```
     15          6           0        2.509179    1.153102    0.038183
     16          1           0        0.013861   -2.720399   -0.059102
     17          1           0       -4.590702   -1.553549    0.035490
     18          1           0       -2.425643   -2.752318   -0.029971
     19          1           0       -2.551575    2.222926    0.071518
     20          1           0       -4.625957    0.944605    0.099629
     21          1           0        4.602928   -1.536996    0.031559
     22          1           0        4.631172    0.962186    0.101134
     23          1           0        2.563646    2.234645    0.077092
     24          6           0       -0.038998    2.726037   -0.070578
     25          1           0       -0.284241    3.149386    0.914161
     26          1           0        0.911159    3.159457   -0.386046
     27          1           0       -0.794382    3.085930   -0.777460
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3929126      0.4479191
0.3397853
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8752763654 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860598332     A.U. after   11 cycles
             Convg  =    0.3389D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000040104    0.000503131   -0.000017784
      2        6          -0.000038515    0.000276652   -0.000013078
      3        6           0.000042090   -0.000129559    0.000009160
      4        6          -0.000155951   -0.000227045    0.000244480
      5        6           0.000346148    0.000136540   -0.000119680
      6        6           0.000176863   -0.000486041   -0.000019043
      7        6          -0.000181629    0.000172149   -0.000154575
      8        6          -0.000203803    0.000109655    0.000028282
      9        6           0.000512582    0.000030631   -0.000229230
     10        6           0.000108267    0.000113159    0.000037277
     11        6          -0.000295923    0.000114244    0.000009482
     12        1           0.000117368   -0.000128130    0.000004608
     13        6          -0.000419584    0.000336973   -0.000038143
     14        6           0.000346326   -0.000403031    0.000005597
     15        6          -0.000389992   -0.000333264   -0.000039540
```

This journal is © The Royal Society of Chemistry 2014

```
     16        1           0.000068703   -0.000151318    0.000147704
     17        1          -0.000027349   -0.000192316    0.000034274
     18        1           0.000058249   -0.000159458    0.000008103
     19        1          -0.000092003    0.000167466   -0.000132876
     20        1          -0.000168592    0.000075784   -0.000047048
     21        1           0.000189201   -0.000073050    0.000050674
     22        1           0.000029028    0.000175372   -0.000074134
     23        1          -0.000077553    0.000198411   -0.000079967
     24        6           0.000093393   -0.000118769    0.000125787
     25        1          -0.000041576    0.000102094   -0.000343845
     26        1          -0.000089393   -0.000117075    0.000274174
     27        1           0.000133749    0.000006793    0.000329340
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000512582 RMS     0.000195410


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000315939 RMS     0.000115020
 Search for a local minimum.
 Step number  32 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    2    3    4    5
6
                                                      7    8   10    9
11
                                                     12   13   14   15
16
                                                     17   18   19   21
20
                                                     23   22   25   24
27
                                                     26   28   29   30
31
                                                     32
 DE= -2.98D-06 DEPred=-6.21D-06 R= 4.80D-01
 Trust test= 4.80D-01 RLast= 8.41D-02 DXMaxT set to 8.41D-02
     Eigenvalues ---   -0.23485   0.00058   0.01496   0.01553
0.01689
     Eigenvalues ---    0.01802   0.01816   0.01860   0.01911
0.01975
     Eigenvalues ---    0.01976   0.02027   0.02073   0.02103
0.02109
     Eigenvalues ---    0.02145   0.02171   0.02223   0.02228
0.02244
     Eigenvalues ---    0.02345   0.02538   0.05682   0.06680
0.10277
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.12256   0.13906   0.15472   0.15900
0.15998
     Eigenvalues ---    0.16000   0.16002   0.16004   0.16047
0.16082
     Eigenvalues ---    0.16313   0.19347   0.21539   0.22014
0.22270
     Eigenvalues ---    0.22645   0.23027   0.24361   0.24571
0.24983
     Eigenvalues ---    0.25476   0.29140   0.29712   0.32603
0.32991
     Eigenvalues ---    0.33595   0.33630   0.33632   0.33682
0.33685
     Eigenvalues ---    0.33806   0.34057   0.34411   0.35666
0.37235
     Eigenvalues ---    0.37591   0.38045   0.38681   0.39625
0.40114
     Eigenvalues ---    0.40748   0.41453   0.42611   0.44872
0.46323
     Eigenvalues ---    0.48732   0.49815   0.51080   0.51435
0.56058
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is  -2.35D-01 should be greater than     0.000000
Eigenvector:
                          D28       D39       D26       D27       D40
```

```
   1                    0.30129  -0.26122   0.24782   0.24429  -
0.22651
                           D37       D25       D38       A48       A12
   1                   -0.20246   0.19082  -0.16775   0.16424  -
0.14438
 Use linear search instead of GDIIS.
 RFO step:  Lambda=-8.71447924D-06 EMin= 2.34848058D-01
 Quartic linear search produced a step of -0.07710.
 Iteration  1 RMS(Cart)=  0.00152612 RMS(Int)=  0.00000146
 Iteration  2 RMS(Cart)=  0.00000199 RMS(Int)=  0.00000019
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000019
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.59028   0.00001   0.00001   0.00001   0.00003
2.59031
    R2        2.69273  -0.00025  -0.00006  -0.00087  -0.00094
2.69179
    R3        2.05346   0.00018   0.00002   0.00076   0.00079
2.05425
    R4        2.70493  -0.00015  -0.00002  -0.00055  -0.00057
2.70436
    R5        2.05545   0.00017   0.00002   0.00066   0.00068
2.05614
    R6        2.73221  -0.00009   0.00004  -0.00031  -0.00027
2.73194
    R7        2.64293  -0.00003  -0.00003  -0.00014  -0.00017
2.64276
    R8        2.71172  -0.00023  -0.00002  -0.00097  -0.00098
2.71073
    R9        2.67953  -0.00007   0.00000  -0.00044  -0.00044
2.67909
   R10        2.59486   0.00016   0.00002   0.00055   0.00057
2.59543
   R11        2.04889   0.00019   0.00001   0.00087   0.00087
2.04977
   R12        2.05397   0.00016   0.00002   0.00063   0.00065
2.05462
   R13        2.64114   0.00009   0.00000   0.00044   0.00044
2.64158
   R14        2.05656   0.00016   0.00002   0.00065   0.00067
2.05723
   R15        2.67812   0.00003   0.00007   0.00045   0.00052
2.67863
   R16        2.86291  -0.00017   0.00000  -0.00099  -0.00098
2.86193
   R17        2.73927  -0.00018  -0.00005  -0.00065  -0.00070
2.73858
   R18        2.71489  -0.00030  -0.00004  -0.00115  -0.00119
2.71369
   R19        2.70654  -0.00020  -0.00005  -0.00081  -0.00086
2.70568
```

This journal is © The Royal Society of Chemistry 2014

R20	2.05543	0.00017	0.00002	0.00067	0.00069
2.05612					
R21	2.58838	0.00004	0.00004	0.00011	0.00015
2.58854					
R22	2.69338	-0.00028	-0.00008	-0.00110	-0.00119
2.69220					
R23	2.05339	0.00019	0.00003	0.00080	0.00083
2.05421					
R24	2.59325	0.00017	0.00005	0.00064	0.00069
2.59394					
R25	2.05395	0.00016	0.00002	0.00062	0.00064
2.05459					
R26	2.04773	0.00021	0.00001	0.00086	0.00087
2.04860					
R27	2.07791	-0.00027	-0.00002	-0.00097	-0.00099
2.07692					
R28	2.06160	-0.00022	0.00001	-0.00094	-0.00093
2.06066					
R29	2.06993	-0.00032	-0.00011	-0.00124	-0.00135
2.06857					
A1	2.08984	0.00008	0.00002	0.00049	0.00050
2.09034					
A2	2.10295	-0.00011	-0.00004	-0.00088	-0.00092
2.10203					
A3	2.09039	0.00003	0.00003	0.00039	0.00042
2.09081					
A4	2.11550	0.00001	0.00002	-0.00001	0.00001
2.11551					
A5	2.10475	-0.00004	-0.00002	-0.00030	-0.00032
2.10443					
A6	2.06292	0.00003	0.00000	0.00031	0.00031
2.06323					
A7	2.08483	-0.00010	-0.00003	-0.00062	-0.00065
2.08418					
A8	2.11446	0.00013	0.00000	0.00079	0.00079
2.11525					
A9	2.08389	-0.00003	0.00003	-0.00017	-0.00014
2.08375					
A10	2.04596	0.00015	0.00000	0.00091	0.00092
2.04687					
A11	2.09674	0.00000	-0.00004	0.00010	0.00006
2.09680					
A12	2.14043	-0.00015	0.00004	-0.00101	-0.00097
2.13947					
A13	2.12309	-0.00006	0.00001	-0.00039	-0.00038
2.12271					
A14	2.08551	0.00002	0.00003	0.00013	0.00016
2.08567					
A15	2.07447	0.00005	-0.00004	0.00026	0.00022
2.07469					
A16	2.10697	-0.00007	-0.00002	-0.00037	-0.00039
2.10658					

A17	2.08514	0.00012	0.00006	0.00083	0.00089
2.08603					
A18	2.09107	-0.00005	-0.00004	-0.00046	-0.00050
2.09057					
A19	2.11873	0.00002	0.00001	0.00014	0.00016
2.11888					
A20	2.08269	-0.00003	-0.00002	-0.00016	-0.00018
2.08252					
A21	2.08173	0.00001	0.00000	0.00002	0.00002
2.08176					
A22	2.08761	0.00005	-0.00001	0.00022	0.00021
2.08783					
A23	2.07883	0.00002	0.00021	-0.00027	-0.00006
2.07877					
A24	2.11670	-0.00007	-0.00020	0.00007	-0.00013
2.11656					
A25	2.08953	-0.00002	0.00003	-0.00021	-0.00018
2.08934					
A26	2.15359	-0.00016	-0.00009	-0.00067	-0.00076
2.15283					
A27	2.04004	0.00017	0.00006	0.00089	0.00095
2.04098					
A28	2.08874	-0.00001	-0.00002	-0.00002	-0.00004
2.08870					
A29	2.10825	0.00010	0.00006	0.00049	0.00055
2.10880					
A30	2.08619	-0.00008	-0.00004	-0.00047	-0.00051
2.08568					
A31	2.06108	0.00004	0.00003	0.00039	0.00042
2.06150					
A32	2.11715	0.00000	0.00000	-0.00006	-0.00006
2.11709					
A33	2.10494	-0.00004	-0.00003	-0.00033	-0.00036
2.10458					
A34	2.08805	0.00007	0.00003	0.00043	0.00046
2.08851					
A35	2.10403	-0.00010	-0.00006	-0.00085	-0.00090
2.10312					
A36	2.09110	0.00004	0.00002	0.00042	0.00044
2.09155					
A37	2.10851	-0.00008	-0.00004	-0.00036	-0.00040
2.10811					
A38	2.08524	0.00011	0.00005	0.00076	0.00081
2.08605					
A39	2.08944	-0.00003	-0.00002	-0.00040	-0.00041
2.08902					
A40	2.12625	-0.00007	-0.00002	-0.00041	-0.00044
2.12581					
A41	2.08893	0.00006	0.00001	0.00043	0.00043
2.08937					
A42	2.06788	0.00002	0.00001	-0.00001	0.00000
2.06788					

This journal is © The Royal Society of Chemistry 2014

A43	1.94843	0.00026	0.00011	0.00218	0.00229	1.95072
A44	1.96341	0.00000	-0.00010	-0.00001	-0.00011	1.96330
A45	1.93996	0.00003	0.00017	0.00010	0.00027	1.94023
A46	1.87576	-0.00019	-0.00011	-0.00158	-0.00169	1.87407
A47	1.87301	-0.00022	-0.00011	-0.00140	-0.00151	1.87150
A48	1.85821	0.00009	0.00003	0.00051	0.00054	1.85876
D1	-0.00145	0.00001	-0.00001	0.00025	0.00024	-0.00121
D2	3.13417	0.00005	0.00002	0.00005	0.00006	3.13423
D3	-3.13838	-0.00002	-0.00004	0.00003	-0.00001	-3.13838
D4	-0.00277	0.00002	-0.00001	-0.00017	-0.00018	-0.00295
D5	0.01127	-0.00005	-0.00004	-0.00007	-0.00012	0.01116
D6	-3.12716	-0.00007	-0.00002	-0.00041	-0.00043	-3.12759
D7	-3.13495	-0.00002	-0.00002	0.00014	0.00012	-3.13482
D8	0.00981	-0.00004	0.00000	-0.00020	-0.00019	0.00961
D9	-0.01464	0.00006	0.00005	0.00028	0.00033	-0.01431
D10	3.12375	0.00008	0.00002	0.00083	0.00085	3.12460
D11	3.13279	0.00003	0.00002	0.00049	0.00051	3.13330
D12	-0.01200	0.00004	-0.00001	0.00103	0.00103	-0.01098
D13	0.02054	-0.00009	-0.00003	-0.00095	-0.00098	0.01956
D14	-3.13180	-0.00002	-0.00001	0.00010	0.00008	-3.13172
D15	-3.11791	-0.00011	0.00000	-0.00149	-0.00149	-3.11940
D16	0.01294	-0.00003	0.00002	-0.00044	-0.00043	0.01251
D17	-3.11890	-0.00011	-0.00004	-0.00063	-0.00067	-3.11957
D18	0.01406	-0.00008	-0.00004	-0.00024	-0.00028	0.01378
D19	0.01949	-0.00010	-0.00007	-0.00008	-0.00015	0.01934
D20	-3.13073	-0.00007	-0.00007	0.00030	0.00023	-3.13050

This journal is © The Royal Society of Chemistry 2014

D21	-0.01125	0.00005	-0.00003	0.00114	0.00112	-0.01013
D22	3.11402	0.00012	0.00004	0.00112	0.00116	3.11518
D23	3.14138	-0.00002	-0.00005	0.00007	0.00002	3.14140
D24	-0.01654	0.00004	0.00002	0.00004	0.00006	-0.01648
D25	-0.04647	0.00018	0.00005	0.00121	0.00126	-0.04521
D26	3.10469	0.00019	0.00022	-0.00099	-0.00077	3.10391
D27	3.08377	0.00026	0.00007	0.00233	0.00240	3.08617
D28	-0.04825	0.00026	0.00024	0.00012	0.00036	-0.04789
D29	-0.00459	0.00002	0.00007	-0.00065	-0.00059	-0.00518
D30	3.13383	0.00003	0.00004	-0.00031	-0.00027	3.13356
D31	-3.12996	-0.00005	0.00000	-0.00063	-0.00063	-3.13059
D32	0.00847	-0.00003	-0.00003	-0.00029	-0.00031	0.00815
D33	-0.01781	0.00008	0.00005	-0.00016	-0.00011	-0.01793
D34	3.12024	0.00009	0.00001	0.00048	0.00049	3.12073
D35	3.13240	0.00005	0.00005	-0.00055	-0.00050	3.13191
D36	-0.01273	0.00006	0.00001	0.00010	0.00011	-0.01262
D37	0.04800	-0.00020	-0.00007	-0.00146	-0.00153	0.04648
D38	-3.08490	-0.00019	-0.00002	-0.00194	-0.00196	-3.08685
D39	-3.10337	-0.00020	-0.00024	0.00079	0.00056	-3.10281
D40	0.04692	-0.00019	-0.00018	0.00031	0.00013	0.04704
D41	1.33455	-0.00005	0.00261	0.00065	0.00326	1.33781
D42	-2.83813	-0.00010	0.00247	0.00018	0.00265	-2.83548
D43	-0.75615	0.00003	0.00256	0.00090	0.00345	-0.75270
D44	-1.79731	-0.00004	0.00277	-0.00159	0.00119	-1.79612
D45	0.31319	-0.00010	0.00264	-0.00206	0.00057	0.31377
D46	2.39517	0.00004	0.00272	-0.00134	0.00138	2.39655

```
   D47       -0.01631   0.00007   0.00002   0.00094   0.00096  -
0.01535
   D48        3.12878   0.00007   0.00006   0.00030   0.00036
3.12914
   D49        3.11715   0.00006  -0.00003   0.00139   0.00136
3.11850
   D50       -0.02095   0.00005   0.00001   0.00075   0.00076  -
0.02019
   D51       -3.13845  -0.00002   0.00000  -0.00049  -0.00050  -
3.13895
   D52        0.02035  -0.00007  -0.00007  -0.00041  -0.00048
0.01987
   D53        0.01161  -0.00001   0.00005  -0.00096  -0.00091
0.01070
   D54       -3.11277  -0.00006  -0.00002  -0.00088  -0.00090  -
3.11367
   D55        0.01239  -0.00003   0.00003  -0.00106  -0.00103
0.01135
   D56       -3.12315  -0.00005   0.00000  -0.00087  -0.00087  -
3.12402
   D57       -3.13274  -0.00002  -0.00001  -0.00042  -0.00043  -
3.13317
   D58        0.01491  -0.00005  -0.00004  -0.00022  -0.00026
0.01465
   D59        0.00150   0.00000   0.00002  -0.00016  -0.00014
0.00136
   D60        3.13873   0.00001   0.00003  -0.00007  -0.00004
3.13869
   D61       -3.13388  -0.00003  -0.00001   0.00004   0.00002  -
3.13386
   D62        0.00335  -0.00002   0.00000   0.00013   0.00013
0.00347
   D63       -0.01142   0.00004   0.00004  -0.00003   0.00001  -
0.01141
   D64        3.12648   0.00005   0.00002   0.00028   0.00029
3.12677
   D65        3.13451   0.00004   0.00003  -0.00012  -0.00010
3.13441
   D66       -0.01078   0.00004   0.00001   0.00018   0.00019  -
0.01059
   D67        0.00449  -0.00004  -0.00007   0.00062   0.00055
0.00504
   D68        3.12907   0.00001   0.00000   0.00054   0.00054
3.12961
   D69       -3.13340  -0.00005  -0.00005   0.00031   0.00026  -
3.13314
   D70       -0.00881   0.00000   0.00002   0.00023   0.00025  -
0.00857
         Item               Value     Threshold  Converged?
 Maximum Force            0.000316     0.000450     YES
 RMS     Force            0.000115     0.000300     YES
 Maximum Displacement     0.007137     0.001800     NO
```

```
 RMS     Displacement     0.001526     0.001200     NO
 Predicted change in Energy=-9.739295D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792981   -5.422680    0.020368
      2          6           0       -3.423019   -5.394250   -0.015715
      3          6           0       -2.707148   -4.155169   -0.030210
      4          6           0       -3.442267   -2.910354   -0.024387
      5          6           0       -4.873662   -2.992379    0.020911
      6          6           0       -5.525274   -4.201154    0.045553
      7          6           0       -1.309048   -4.126509   -0.046704
      8          6           0       -2.748854   -1.674071   -0.050667
      9          6           0       -1.331610   -1.664997   -0.026965
     10          6           0       -0.605090   -2.918897   -0.034630
     11          6           0        0.826596   -2.904295   -0.026120
     12          1           0        1.349189   -3.858522   -0.040215
     13          6           0        1.526087   -1.727010    0.006299
     14          6           0        0.821760   -0.488952    0.033870
     15          6           0       -0.550474   -0.460737    0.014897
     16          1           0       -0.756764   -5.064538   -0.061605
     17          1           0       -5.323946   -6.371149    0.034023
     18          1           0       -2.850385   -6.319347   -0.028366
     19          1           0       -5.460218   -2.080480    0.051608
     20          1           0       -6.611386   -4.228405    0.087385
     21          1           0        2.613086   -1.731164    0.015110
     22          1           0        1.379110    0.443724    0.073596
     23          1           0       -1.048267    0.501703    0.048474
     24          6           0       -3.542631   -0.385013   -0.093764
     25          1           0       -3.967210   -0.134766    0.888599
     26          1           0       -2.940003    0.465397   -0.414289
     27          1           0       -4.377021   -0.457999   -0.798538
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1          2          3          4          5
    1  C    0.000000
    2  C    1.370732   0.000000
    3  C    2.441279   1.431084   0.000000
    4  C    2.852755   2.483985   1.445682   0.000000
    5  C    2.431640   2.806188   2.459365   1.434459   0.000000
    6  C    1.424435   2.417997   2.819519   2.451525   1.373441
    7  C    3.717841   2.465156   1.398491   2.455637   3.741296
    8  C    4.270313   3.780933   2.481533   1.417713   2.501574
    9  C    5.109160   4.275681   2.844833   2.450673   3.782906
   10  C    4.879588   3.750793   2.438655   2.837209   4.269567
   11  C    6.158252   4.925364   3.748607   4.268868   5.701133
```

This journal is © The Royal Society of Chemistry 2014

12	H	6.338494	5.013285	4.067182	4.884396	6.283138
13	C	7.320436	6.159771	4.880324	5.107424	6.523662
14	C	7.474434	6.487106	5.089051	4.903927	6.221346
15	C	6.528382	5.708940	4.278096	3.790071	5.009911
16	H	4.052903	2.686955	2.152193	3.442937	4.609718
17	H	1.087062	2.137833	3.429625	3.939699	3.408667
18	H	2.140109	1.088060	2.168914	3.459996	3.894200
19	H	3.408297	3.890473	3.448249	2.183253	1.084689
20	H	2.176553	3.396396	3.906695	3.434103	2.133509
21	H	8.275092	7.060716	5.846601	6.169226	7.592240
22	H	8.515411	7.559785	6.152893	5.874105	7.134896
23	H	7.008708	6.356557	4.944141	4.168774	5.181025
24	C	5.191771	5.011272	3.862142	2.528287	2.929702
25	H	5.421970	5.364335	4.312262	2.968670	3.120976
26	H	6.188045	5.893015	4.642345	3.435111	3.985555
27	H	5.048929	5.088173	4.128906	2.736260	2.709471

		6	7	8	9	10
6	C	0.000000				
7	C	4.217896	0.000000			
8	C	3.755518	2.843855	0.000000		
9	C	4.901446	2.461695	1.417471	0.000000	
10	C	5.085158	1.397866	2.479027	1.449192	0.000000
11	C	6.483305	2.460734	3.781256	2.488717	1.431786
12	H	6.883531	2.671719	4.643909	3.463872	2.168440
13	C	7.472926	3.714619	4.275648	2.858563	2.442168
14	C	7.352919	4.216474	3.763102	2.454339	2.818727
15	C	6.224170	3.743944	2.511842	1.436025	2.459266
16	H	4.847226	1.088640	3.932405	3.447974	2.151164
17	H	2.179345	4.600470	5.357314	6.171737	5.847252
18	H	3.412805	2.680409	4.646439	4.895882	4.074856
19	H	2.121680	4.629051	2.743560	4.150205	4.927743
20	H	1.087258	5.305011	4.632800	5.870279	6.148601
21	H	8.504980	4.596155	5.362648	3.945475	3.430720
22	H	8.321429	5.303555	4.641182	3.435813	3.905890
23	H	6.493109	4.636530	2.763298	2.186449	3.450191
24	C	4.302698	4.357740	1.514466	2.555668	3.879848
25	H	4.435516	4.886167	2.176252	3.182177	4.461793
26	H	5.354603	4.886792	2.178550	2.697318	4.129093
27	H	4.005269	4.841041	2.165426	3.365516	4.568046

		11	12	13	14	15
11	C	0.000000				
12	H	1.088050	0.000000			
13	C	1.369794	2.139346	0.000000		
14	C	2.416092	3.411403	1.424649	0.000000	
15	C	2.805171	3.893161	2.432206	1.372655	0.000000
16	H	2.678608	2.426926	4.044145	4.841161	4.609056
17	H	7.060585	7.130886	8.275974	8.507052	7.597327
18	H	5.018245	4.867465	6.343837	6.890720	6.294027
19	H	6.341037	7.038315	6.995387	6.480472	5.170155
20	H	7.555775	7.970185	8.513637	8.320939	7.136892
21	H	2.137635	2.475106	1.087043	2.179976	3.409120
22	H	3.394767	4.303855	2.176745	1.087245	2.131850

23	H	3.888637	4.976668	3.405325	2.116273	1.084073
24	C	5.043957	5.999836	5.244318	4.367494	2.995087
25	H	5.611380	6.556916	5.787055	4.877524	3.541708
26	H	5.068804	6.101916	4.992946	3.906724	2.598418
27	H	5.801606	6.702842	6.091374	5.265091	3.912052

		16	17	18	19	20
16	H	0.000000				
17	H	4.751371	0.000000			
18	H	2.441085	2.474890	0.000000		
19	H	5.571346	4.292869	4.978516	0.000000	
20	H	5.915903	2.500340	4.304714	2.437222	0.000000
21	H	4.740586	9.193818	7.134622	8.080940	9.556795
22	H	5.909415	9.559027	7.977352	7.290301	9.256187
23	H	5.574955	8.094302	7.055512	5.112043	7.302310
24	C	5.446103	6.246858	5.974931	2.563762	4.921558
25	H	5.959236	6.439216	6.351155	2.591414	4.938774
26	H	5.955762	7.254138	6.796302	3.612482	5.980176
27	H	5.905043	6.046087	6.105668	2.128029	4.471376

		21	22	23	24	25
21	H	0.000000				
22	H	2.501251	0.000000			
23	H	4.288626	2.428199	0.000000		
24	C	6.302130	4.993831	2.651104	0.000000	
25	H	6.827281	5.438935	3.103407	1.099058	0.000000
26	H	5.987159	4.346635	1.947854	1.090456	1.764332
27	H	7.151544	5.891245	3.566380	1.094641	1.766029

		26	27
26	H	0.000000	
27	H	1.750808	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.654677	-1.000297	0.024035
2	6	0	-2.456378	-1.664856	-0.012658
3	6	0	-1.214275	-0.954160	-0.022330
4	6	0	-1.223281	0.491449	-0.010888
5	6	0	-2.501651	1.140565	0.034829
6	6	0	-3.672990	0.423690	0.054740
7	6	0	0.008424	-1.632755	-0.039448
8	6	0	-0.001973	1.211072	-0.032345
9	6	0	1.227350	0.505763	-0.009359
10	6	0	1.224356	-0.943365	-0.022677
11	6	0	2.468966	-1.651104	-0.014869
12	1	0	2.440521	-2.738626	-0.033250

```
     13          6           0        3.665745   -0.985754    0.022121
     14          6           0        3.679914    0.438439    0.055267
     15          6           0        2.508243    1.153310    0.037143
     16          1           0        0.013789   -2.721214   -0.058583
     17          1           0       -4.590766   -1.552873    0.033990
     18          1           0       -2.426924   -2.752387   -0.029499
     19          1           0       -2.549807    2.223624    0.069667
     20          1           0       -4.625399    0.946432    0.097037
     21          1           0        4.603036   -1.536281    0.030336
     22          1           0        4.630771    0.963885    0.098613
     23          1           0        2.562220    2.235375    0.075028
     24          6           0       -0.039332    2.724619   -0.069605
     25          1           0       -0.281974    3.150673    0.914027
     26          1           0        0.909860    3.157594   -0.386876
     27          1           0       -0.795977    3.084099   -0.774234
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3936062      0.4479929
0.3398607
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9741880147 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860602337     A.U. after   10 cycles
            Convg  =    0.6395D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6          -0.000077460   -0.000119192   -0.000006440
      2          6           0.000089834   -0.000089974    0.000010851
      3          6           0.000074732   -0.000052020   -0.000005407
      4          6           0.000021996    0.000040112    0.000190294
      5          6          -0.000222749   -0.000006037   -0.000018012
      6          6          -0.000101777    0.000068865   -0.000035629
      7          6           0.000049085   -0.000014187   -0.000117898
      8          6           0.000047850    0.000048693   -0.000031184
      9          6          -0.000122597    0.000038134   -0.000217579
     10          6          -0.000043363   -0.000119857   -0.000002146
     11          6           0.000031067   -0.000151172    0.000026349
     12          1          -0.000018631    0.000077637   -0.000006347
     13          6           0.000168841    0.000016365   -0.000022669
     14          6          -0.000007312    0.000133457   -0.000014455
     15          6           0.000010623    0.000127273    0.000045538
     16          1          -0.000032794    0.000064707    0.000164175
     17          1           0.000051719    0.000074199    0.000036372
     18          1          -0.000055996    0.000054486   -0.000003609
     19          1           0.000066906   -0.000160035   -0.000105153
     20          1           0.000069626    0.000006315   -0.000065200
     21          1          -0.000095381   -0.000013359    0.000052154
     22          1          -0.000039596   -0.000056866   -0.000091523
     23          1           0.000083991   -0.000106414   -0.000066093
     24          6           0.000177387    0.000042987    0.000199511
     25          1          -0.000086250   -0.000029062    0.000090779
     26          1           0.000079757    0.000121703    0.000058203
     27          1          -0.000119507    0.000003240   -0.000064883
```

This journal is © The Royal Society of Chemistry 2014

```
 ----------------------------------------------------------------------
 Cartesian Forces:  Max     0.000222749 RMS     0.000087992


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000240543 RMS     0.000075052
 Search for a local minimum.
 Step number  33 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points    2    3    4    5
6
                                                      7    8   10    9
11
                                                     12   13   14   15
16
                                                     17   18   19   21
20
                                                     23   22   25   24
27
                                                     26   28   29   30
31
                                                     32   33
 DE= -4.01D-06 DEPred=-9.74D-06 R= 4.11D-01
 Trust test= 4.11D-01 RLast= 1.03D-02 DXMaxT set to 8.41D-02
 Use linear search instead of GDIIS.
     Eigenvalues ---    0.00000   0.01438   0.01481   0.01649
0.01800
     Eigenvalues ---    0.01816   0.01836   0.01903   0.01967
0.01975
     Eigenvalues ---    0.01992   0.02035   0.02074   0.02107
0.02126
     Eigenvalues ---    0.02145   0.02183   0.02223   0.02243
0.02334
     Eigenvalues ---    0.02403   0.02960   0.06521   0.06735
0.11814
     Eigenvalues ---    0.12576   0.15542   0.15754   0.15949
0.15999
     Eigenvalues ---    0.16000   0.16003   0.16010   0.16060
0.16097
     Eigenvalues ---    0.16459   0.21383   0.21942   0.22053
0.22589
     Eigenvalues ---    0.23019   0.23426   0.24387   0.24742
0.25241
     Eigenvalues ---    0.26040   0.30010   0.31972   0.33235
0.33594
     Eigenvalues ---    0.33625   0.33631   0.33682   0.33688
0.33710
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.34024   0.34256   0.35034   0.35849
0.37273
     Eigenvalues ---    0.37971   0.38372   0.38918   0.39544
0.40183
     Eigenvalues ---    0.40913   0.41969   0.43316   0.45176
0.47981
     Eigenvalues ---    0.48905   0.49836   0.51204   0.51414
0.63823
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-1.30084261D-04 EMin= 2.54201395D-08
 Quartic linear search produced a step of -0.11452.
 Maximum step size (   0.084) exceeded in Quadratic search.
    -- Step size scaled by   0.090
 Iteration  1 RMS(Cart)=  0.00978447 RMS(Int)=  0.00015529
 Iteration  2 RMS(Cart)=  0.00016089 RMS(Int)=  0.00000025
 Iteration  3 RMS(Cart)=  0.00000003 RMS(Int)=  0.00000024
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.59031   0.00003   0.00000   0.00018   0.00017
2.59048
    R2        2.69179   0.00003   0.00011  -0.00008   0.00003
2.69182
```

This journal is © The Royal Society of Chemistry 2014

R3	2.05425	-0.00009	-0.00009	0.00003	-0.00006
2.05419					
R4	2.70436	0.00004	0.00007	-0.00012	-0.00005
2.70431					
R5	2.05614	-0.00008	-0.00008	0.00004	-0.00004
2.05609					
R6	2.73194	0.00013	0.00003	-0.00049	-0.00046
2.73148					
R7	2.64276	-0.00003	0.00002	0.00002	0.00004
2.64281					
R8	2.71073	0.00018	0.00011	-0.00025	-0.00014
2.71059					
R9	2.67909	0.00023	0.00005	-0.00010	-0.00005
2.67904					
R10	2.59543	-0.00003	-0.00007	0.00007	0.00001
2.59543					
R11	2.04977	-0.00017	-0.00010	0.00011	0.00002
2.04978					
R12	2.05462	-0.00007	-0.00007	0.00005	-0.00002
2.05460					
R13	2.64158	-0.00008	-0.00005	-0.00013	-0.00018
2.64141					
R14	2.05723	-0.00007	-0.00008	0.00003	-0.00004
2.05719					
R15	2.67863	0.00001	-0.00006	0.00009	0.00003
2.67866					
R16	2.86193	0.00008	0.00011	0.00023	0.00034
2.86227					
R17	2.73858	0.00009	0.00008	0.00050	0.00058
2.73916					
R18	2.71369	0.00008	0.00014	0.00030	0.00043
2.71413					
R19	2.70568	0.00005	0.00010	0.00006	0.00016
2.70584					
R20	2.05612	-0.00008	-0.00008	0.00003	-0.00005
2.05607					
R21	2.58854	0.00006	-0.00002	-0.00009	-0.00011
2.58843					
R22	2.69220	0.00006	0.00014	-0.00007	0.00007
2.69226					
R23	2.05421	-0.00010	-0.00009	0.00002	-0.00008
2.05414					
R24	2.59394	-0.00002	-0.00008	-0.00011	-0.00019
2.59375					
R25	2.05459	-0.00007	-0.00007	0.00005	-0.00003
2.05457					
R26	2.04860	-0.00013	-0.00010	-0.00017	-0.00027
2.04833					
R27	2.07692	0.00011	0.00011	-0.00005	0.00006
2.07698					
R28	2.06066	0.00012	0.00011	-0.00053	-0.00043
2.06024					

This journal is © The Royal Society of Chemistry 2014

R29	2.06857	0.00013	0.00016	0.00058	0.00073
2.06931					
A1	2.09034	0.00000	-0.00006	0.00018	0.00012
2.09046					
A2	2.10203	-0.00001	0.00011	-0.00019	-0.00008
2.10194					
A3	2.09081	0.00001	-0.00005	0.00001	-0.00004
2.09077					
A4	2.11551	0.00002	0.00000	-0.00006	-0.00006
2.11545					
A5	2.10443	-0.00003	0.00004	-0.00011	-0.00007
2.10436					
A6	2.06323	0.00001	-0.00004	0.00017	0.00013
2.06336					
A7	2.08418	0.00003	0.00007	-0.00025	-0.00018
2.08400					
A8	2.11525	-0.00005	-0.00009	0.00060	0.00051
2.11577					
A9	2.08375	0.00002	0.00002	-0.00035	-0.00033
2.08342					
A10	2.04687	-0.00010	-0.00011	0.00055	0.00045
2.04732					
A11	2.09680	-0.00005	-0.00001	0.00059	0.00059
2.09739					
A12	2.13947	0.00015	0.00011	-0.00114	-0.00103
2.13844					
A13	2.12271	0.00005	0.00004	-0.00021	-0.00017
2.12254					
A14	2.08567	0.00000	-0.00002	-0.00042	-0.00044
2.08523					
A15	2.07469	-0.00006	-0.00003	0.00064	0.00062
2.07531					
A16	2.10658	0.00001	0.00004	-0.00018	-0.00014
2.10644					
A17	2.08603	0.00000	-0.00010	0.00012	0.00001
2.08604					
A18	2.09057	-0.00001	0.00006	0.00007	0.00013
2.09070					
A19	2.11888	0.00003	-0.00002	0.00002	0.00001
2.11889					
A20	2.08252	-0.00001	0.00002	0.00002	0.00004
2.08256					
A21	2.08176	-0.00002	0.00000	-0.00004	-0.00005
2.08171					
A22	2.08783	-0.00005	-0.00002	0.00000	-0.00002
2.08780					
A23	2.07877	0.00016	0.00001	-0.00293	-0.00292
2.07585					
A24	2.11656	-0.00012	0.00002	0.00293	0.00294
2.11951					
A25	2.08934	0.00002	0.00002	-0.00055	-0.00053
2.08881					

A26	2.15283	0.00002	0.00009	0.00101	0.00110	2.15393
A27	2.04098	-0.00004	-0.00011	-0.00046	-0.00057	2.04042
A28	2.08870	0.00003	0.00001	0.00036	0.00037	2.08906
A29	2.10880	-0.00003	-0.00006	-0.00041	-0.00047	2.10833
A30	2.08568	0.00001	0.00006	0.00005	0.00010	2.08579
A31	2.06150	0.00002	-0.00005	-0.00004	-0.00008	2.06142
A32	2.11709	0.00000	0.00001	0.00018	0.00019	2.11728
A33	2.10458	-0.00002	0.00004	-0.00014	-0.00010	2.10448
A34	2.08851	-0.00001	-0.00005	-0.00010	-0.00015	2.08835
A35	2.10312	-0.00001	0.00010	-0.00003	0.00007	2.10320
A36	2.09155	0.00001	-0.00005	0.00013	0.00008	2.09163
A37	2.10811	0.00000	0.00005	0.00003	0.00008	2.10819
A38	2.08605	0.00001	-0.00009	0.00007	-0.00003	2.08602
A39	2.08902	-0.00001	0.00005	-0.00010	-0.00005	2.08897
A40	2.12581	0.00004	0.00005	0.00031	0.00036	2.12617
A41	2.08937	0.00001	-0.00005	0.00028	0.00023	2.08959
A42	2.06788	-0.00004	0.00000	-0.00058	-0.00058	2.06730
A43	1.95072	-0.00007	-0.00026	-0.00011	-0.00038	1.95034
A44	1.96330	0.00004	0.00001	0.00188	0.00189	1.96519
A45	1.94023	0.00004	-0.00003	-0.00158	-0.00161	1.93862
A46	1.87407	-0.00001	0.00019	0.00018	0.00037	1.87444
A47	1.87150	-0.00003	0.00017	-0.00073	-0.00056	1.87094
A48	1.85876	0.00002	-0.00006	0.00032	0.00026	1.85902
D1	-0.00121	0.00000	-0.00003	0.00015	0.00012	-0.00109
D2	3.13423	0.00004	-0.00001	0.00045	0.00044	3.13467
D3	-3.13838	-0.00002	0.00000	-0.00023	-0.00023	-3.13861

This journal is © The Royal Society of Chemistry 2014

D4	-0.00295	0.00002	0.00002	0.00008	0.00010	-0.00285
D5	0.01116	-0.00005	0.00001	-0.00039	-0.00038	0.01078
D6	-3.12759	-0.00006	0.00005	-0.00057	-0.00052	-3.12812
D7	-3.13482	-0.00003	-0.00001	-0.00002	-0.00003	-3.13486
D8	0.00961	-0.00003	0.00002	-0.00020	-0.00018	0.00943
D9	-0.01431	0.00006	-0.00004	0.00052	0.00048	-0.01383
D10	3.12460	0.00006	-0.00010	0.00097	0.00087	3.12548
D11	3.13330	0.00002	-0.00006	0.00022	0.00017	3.13346
D12	-0.01098	0.00002	-0.00012	0.00068	0.00056	-0.01042
D13	0.01956	-0.00007	0.00011	-0.00092	-0.00080	0.01876
D14	-3.13172	-0.00002	-0.00001	-0.00010	-0.00010	-3.13182
D15	-3.11940	-0.00007	0.00017	-0.00136	-0.00119	-3.12059
D16	0.01251	-0.00002	0.00005	-0.00054	-0.00049	0.01202
D17	-3.11957	-0.00009	0.00008	-0.00143	-0.00135	-3.12092
D18	0.01378	-0.00008	0.00003	-0.00072	-0.00069	0.01309
D19	0.01934	-0.00009	0.00002	-0.00098	-0.00096	0.01838
D20	-3.13050	-0.00008	-0.00003	-0.00027	-0.00030	-3.13079
D21	-0.01013	0.00002	-0.00013	0.00070	0.00057	-0.00956
D22	3.11518	0.00009	-0.00013	0.00108	0.00094	3.11612
D23	3.14140	-0.00003	0.00000	-0.00016	-0.00016	3.14124
D24	-0.01648	0.00004	-0.00001	0.00022	0.00022	-0.01626
D25	-0.04521	0.00015	-0.00014	0.00172	0.00158	-0.04363
D26	3.10391	0.00020	0.00009	0.00112	0.00121	3.10512
D27	3.08617	0.00020	-0.00027	0.00260	0.00232	3.08849
D28	-0.04789	0.00024	-0.00004	0.00200	0.00195	-0.04594
D29	-0.00518	0.00004	0.00007	-0.00005	0.00001	-0.00516

This journal is © The Royal Society of Chemistry 2014

D30	3.13356	0.00005	0.00003	0.00013	0.00016	3.13372
D31	-3.13059	-0.00003	0.00007	-0.00042	-0.00035	-3.13094
D32	0.00815	-0.00002	0.00004	-0.00024	-0.00020	0.00795
D33	-0.01793	0.00008	0.00001	0.00127	0.00129	-0.01664
D34	3.12073	0.00007	-0.00006	0.00139	0.00133	3.12207
D35	3.13191	0.00007	0.00006	0.00057	0.00062	3.13253
D36	-0.01262	0.00006	-0.00001	0.00068	0.00067	-0.01195
D37	0.04648	-0.00016	0.00017	-0.00145	-0.00127	0.04521
D38	-3.08685	-0.00014	0.00022	-0.00182	-0.00159	-3.08844
D39	-3.10281	-0.00021	-0.00006	-0.00086	-0.00092	-3.10373
D40	0.04704	-0.00018	-0.00001	-0.00123	-0.00124	0.04580
D41	1.33781	-0.00008	-0.00037	-0.03504	-0.03541	1.30240
D42	-2.83548	-0.00011	-0.00030	-0.03355	-0.03385	-2.86934
D43	-0.75270	-0.00002	-0.00040	-0.03296	-0.03335	-0.78605
D44	-1.79612	-0.00003	-0.00014	-0.03564	-0.03577	-1.83189
D45	0.31377	-0.00006	-0.00007	-0.03415	-0.03421	0.27955
D46	2.39655	0.00002	-0.00016	-0.03356	-0.03371	2.36284
D47	-0.01535	0.00005	-0.00011	-0.00005	-0.00016	-0.01551
D48	3.12914	0.00006	-0.00004	-0.00016	-0.00021	3.12894
D49	3.11850	0.00003	-0.00016	0.00030	0.00015	3.11865
D50	-0.02019	0.00004	-0.00009	0.00019	0.00010	-0.02009
D51	-3.13895	-0.00001	0.00006	0.00027	0.00032	-3.13862
D52	0.01987	-0.00007	0.00006	0.00034	0.00040	0.02027
D53	0.01070	0.00001	0.00010	-0.00009	0.00001	0.01071
D54	-3.11367	-0.00004	0.00010	-0.00002	0.00008	-3.11359
D55	0.01135	-0.00001	0.00012	-0.00009	0.00002	0.01138

```
   D56       -3.12402  -0.00003   0.00010  -0.00024  -0.00014  -
3.12416
   D57       -3.13317  -0.00002   0.00005   0.00002   0.00007  -
3.13310
   D58        0.01465  -0.00005   0.00003  -0.00012  -0.00009
0.01455
   D59        0.00136   0.00000   0.00002  -0.00004  -0.00002
0.00133
   D60        3.13869   0.00001   0.00000   0.00004   0.00005
3.13874
   D61       -3.13386  -0.00002   0.00000  -0.00019  -0.00019  -
3.13405
   D62        0.00347  -0.00002  -0.00001  -0.00010  -0.00012
0.00336
   D63       -0.01141   0.00005   0.00000   0.00014   0.00014  -
0.01127
   D64        3.12677   0.00005  -0.00003   0.00019   0.00015
3.12692
   D65        3.13441   0.00004   0.00001   0.00006   0.00007
3.13448
   D66       -0.01059   0.00004  -0.00002   0.00010   0.00008  -
0.01051
   D67        0.00504  -0.00006  -0.00006  -0.00007  -0.00013
0.00490
   D68        3.12961   0.00000  -0.00006  -0.00014  -0.00020
3.12941
   D69       -3.13314  -0.00006  -0.00003  -0.00012  -0.00015  -
3.13329
   D70       -0.00857   0.00000  -0.00003  -0.00019  -0.00021  -
0.00878
         Item               Value     Threshold  Converged?
 Maximum Force            0.000241     0.000450     YES
 RMS     Force            0.000075     0.000300     YES
 Maximum Displacement     0.065969     0.001800     NO
 RMS     Displacement     0.009784     0.001200     NO
 Predicted change in Energy=-1.181150D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793130   -5.421262    0.021608
      2          6           0       -3.423034   -5.393591   -0.013434
      3          6           0       -2.706573   -4.154885   -0.028112
      4          6           0       -3.441193   -2.910055   -0.022992
      5          6           0       -4.872623   -2.991002    0.020790
      6          6           0       -5.524943   -4.199401    0.045351
      7          6           0       -1.308452   -4.126189   -0.044589
```

8	6	0	-2.748131	-1.673603	-0.049319
9	6	0	-1.330851	-1.664211	-0.026933
10	6	0	-0.604585	-2.918616	-0.034304
11	6	0	0.827200	-2.904611	-0.027397
12	1	0	1.349281	-3.859093	-0.041302
13	6	0	1.527413	-1.727771	0.003098
14	6	0	0.823663	-0.489333	0.030219
15	6	0	-0.548477	-0.460412	0.012882
16	1	0	-0.756104	-5.064166	-0.058683
17	1	0	-5.324528	-6.369451	0.035202
18	1	0	-2.850975	-6.319027	-0.025389
19	1	0	-5.458155	-2.078387	0.050007
20	1	0	-6.611104	-4.226158	0.085864
21	1	0	2.614380	-1.732500	0.010658
22	1	0	1.381502	0.443104	0.068273
23	1	0	-1.045094	0.502482	0.046256
24	6	0	-3.546126	-0.386911	-0.091517
25	1	0	-4.000335	-0.157308	0.882637
26	1	0	-2.940257	0.472543	-0.379380
27	1	0	-4.360198	-0.452198	-0.820978

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370823	0.000000			
3	C	2.441292	1.431057	0.000000		
4	C	2.852348	2.483621	1.445440	0.000000	
5	C	2.431560	2.806227	2.459428	1.434385	0.000000
6	C	1.424451	2.418174	2.819679	2.451346	1.373445
7	C	3.718142	2.465509	1.398513	2.455206	3.741155
8	C	4.269895	3.780885	2.481720	1.417688	2.500784
9	C	5.109321	4.276176	2.845359	2.450650	3.782433
10	C	4.879577	3.750945	2.438596	2.836644	4.269007
11	C	6.158250	4.925414	3.748431	4.268399	5.700681
12	H	6.338260	5.013028	4.066647	4.883610	6.282477
13	C	7.320621	6.159987	4.880419	5.107399	6.523536
14	C	7.474782	6.487533	5.089424	4.904256	6.221423
15	C	6.528950	5.709643	4.278806	3.790757	5.010208
16	H	4.053584	2.687579	2.152221	3.442554	4.609778
17	H	1.087028	2.137837	3.429578	3.939259	3.408569
18	H	2.140130	1.088038	2.168956	3.459690	3.894219
19	H	3.408501	3.890542	3.448064	2.182918	1.084697
20	H	2.176564	3.396550	3.906844	3.433993	2.133579
21	H	8.275161	7.060774	5.846536	6.169095	7.592044
22	H	8.515811	7.560241	6.153303	5.874554	7.135083
23	H	7.009930	6.357817	4.945412	4.170311	5.182186
24	C	5.187727	5.008802	3.860893	2.526255	2.924637
25	H	5.392505	5.343676	4.299291	2.951341	3.087635
26	H	6.191193	5.897331	4.646620	3.438010	3.986266
27	H	5.058556	5.093895	4.131949	2.742701	2.723359

		6	7	8	9	10
6	C	0.000000				

This journal is © The Royal Society of Chemistry 2014

7	C	4.218086	0.000000			
8	C	3.754903	2.843919	0.000000		
9	C	4.901308	2.462143	1.417488	0.000000	
10	C	5.084946	1.397772	2.478925	1.449499	0.000000
11	C	6.483170	2.460397	3.781382	2.489131	1.431870
12	H	6.883187	2.671122	4.643836	3.464219	2.168441
13	C	7.473049	3.714406	4.276208	2.859128	2.442320
14	C	7.353205	4.216424	3.763846	2.454696	2.818771
15	C	6.224652	3.744167	2.512803	1.436254	2.459297
16	H	4.847728	1.088617	3.932451	3.448338	2.151031
17	H	2.179309	4.600811	5.356860	6.171920	5.847303
18	H	3.412906	2.681097	4.646623	4.896742	4.075431
19	H	2.122070	4.628442	2.741887	4.148746	4.926482
20	H	1.087245	5.305198	4.632102	5.870039	6.148363
21	H	8.505021	4.595803	5.363170	3.946001	3.430835
22	H	8.321800	5.303492	4.641998	3.436088	3.905922
23	H	6.494362	4.637047	2.764926	2.186681	3.450283
24	C	4.297619	4.357934	1.514647	2.557950	3.881426
25	H	4.400453	4.884465	2.176168	3.197533	4.471769
26	H	5.356123	4.891136	2.179861	2.698170	4.132118
27	H	4.018543	4.838817	2.164728	3.358039	4.561436

		11	12	13	14	15
11	C	0.000000				
12	H	1.088024	0.000000			
13	C	1.369738	2.139214	0.000000		
14	C	2.415968	3.411256	1.424685	0.000000	
15	C	2.805034	3.893000	2.432204	1.372554	0.000000
16	H	2.677967	2.425932	4.043489	4.840730	4.608989
17	H	7.060651	7.130741	8.276190	8.507412	7.597888
18	H	5.018685	4.867615	6.344346	6.891399	6.294944
19	H	6.339899	7.037075	6.994518	6.479716	5.169541
20	H	7.555638	7.969857	8.513768	8.321220	7.137339
21	H	2.137593	2.474989	1.087003	2.180026	3.409088
22	H	3.394643	4.303712	2.176748	1.087231	2.131720
23	H	3.888341	4.976347	3.404950	2.115705	1.083931
24	C	5.046673	6.001964	5.248586	4.372684	3.000366
25	H	5.628581	6.570788	5.813427	4.909971	3.572627
26	H	5.071764	6.105530	4.994771	3.906413	2.597091
27	H	5.792512	6.694249	6.080308	5.253411	3.901872

		16	17	18	19	20
16	H	0.000000				
17	H	4.752166	0.000000			
18	H	2.442185	2.474809	0.000000		
19	H	5.570994	4.293170	4.978564	0.000000	
20	H	5.916432	2.500310	4.304770	2.437929	0.000000
21	H	4.739722	9.193921	7.134958	8.080037	9.556858
22	H	5.908934	9.559437	7.978035	7.289660	9.256568
23	H	5.575132	8.095501	7.056863	5.112338	7.303565
24	C	5.446285	6.242561	5.973074	2.556751	4.915829
25	H	5.957212	6.407991	6.333428	2.551285	4.899642
26	H	5.960580	7.257376	6.801374	3.609907	5.980749
27	H	5.902613	6.056143	6.109861	2.146769	4.486838

		21	22	23	24	25
21	H	0.000000				
22	H	2.501312	0.000000			
23	H	4.288142	2.427422	0.000000		
24	C	6.306574	4.999597	2.658036	0.000000	
25	H	6.855365	5.476116	3.141385	1.099090	0.000000
26	H	5.989017	4.344980	1.942602	1.090230	1.764416
27	H	7.139715	5.878728	3.557164	1.095029	1.766003

		26	27
26	H	0.000000	
27	H	1.751110	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.653869	-1.001496	0.023145
2	6	0	-2.455365	-1.665965	-0.011902
3	6	0	-1.213419	-0.955042	-0.021059
4	6	0	-1.222976	0.490326	-0.010251
5	6	0	-2.501298	1.139522	0.033301
6	6	0	-3.672582	0.422530	0.052470
7	6	0	0.009787	-1.632782	-0.037538
8	6	0	-0.002368	1.211104	-0.031064
9	6	0	1.227617	0.506894	-0.008771
10	6	0	1.225144	-0.942544	-0.021870
11	6	0	2.470022	-1.649995	-0.015036
12	1	0	2.441757	-2.737499	-0.033298
13	6	0	3.666732	-0.984571	0.020702
14	6	0	3.680603	0.439670	0.053479
15	6	0	2.508887	1.154299	0.036402
16	1	0	0.015984	-2.721226	-0.055917
17	1	0	-4.589820	-1.554252	0.032511
18	1	0	-2.425829	-2.753481	-0.028088
19	1	0	-2.548963	2.222657	0.066691
20	1	0	-4.625160	0.945078	0.092966
21	1	0	4.604079	-1.534935	0.028137
22	1	0	4.631385	0.965315	0.095687
23	1	0	2.563352	2.236202	0.074168
24	6	0	-0.045574	2.724699	-0.067380
25	1	0	-0.325008	3.147612	0.907844
26	1	0	0.910768	3.164396	-0.351418
27	1	0	-0.780597	3.080241	-0.797051

Rotational constants (GHZ): 1.3936456 0.4479710
0.3398411

This journal is © The Royal Society of Chemistry 2014

```
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9635635440 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
```

```
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860612502     A.U. after   10 cycles
             Convg  =    0.9252D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000041538   -0.000079717   -0.000021953
      2        6           0.000061555   -0.000078987    0.000026278
      3        6           0.000030230   -0.000061934   -0.000007887
      4        6          -0.000010772    0.000005375    0.000155617
      5        6          -0.000177277   -0.000001736    0.000001792
      6        6          -0.000096713    0.000031804   -0.000035386
      7        6           0.000034504   -0.000036813   -0.000147240
      8        6           0.000039402    0.000130281    0.000114801
      9        6          -0.000065474    0.000076003   -0.000231021
     10        6          -0.000032800   -0.000049909    0.000003288
     11        6           0.000024980   -0.000127920    0.000041513
     12        1          -0.000019433    0.000057334    0.000000572
     13        6           0.000122745    0.000013951   -0.000037807
     14        6           0.000025616    0.000094597   -0.000014217
     15        6          -0.000100407    0.000037319    0.000059603
     16        1          -0.000024229    0.000051311    0.000152359
     17        1           0.000040061    0.000054438    0.000039487
     18        1          -0.000044119    0.000042252    0.000000645
     19        1           0.000031874   -0.000181880   -0.000133125
     20        1           0.000060056    0.000004005   -0.000062505
     21        1          -0.000070367   -0.000012703    0.000049895
     22        1          -0.000041113   -0.000046779   -0.000086220
     23        1           0.000003799   -0.000036436   -0.000108960
     24        6           0.000217610   -0.000024851    0.000162047
     25        1           0.000019662   -0.000025127    0.000002531
     26        1           0.000127992    0.000144751    0.000119428
     27        1          -0.000115845    0.000021373   -0.000043533
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000231021 RMS     0.000082308
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000432406 RMS     0.000096206
 Search for a local minimum.
 Step number  34 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   13   14   15   16
17
                                                     18   19   21   20
23
                                                     22   25   24   27
26
                                                     28   29   30   31
32
                                                     33   34
 DE= -1.02D-05 DEPred=-1.18D-05 R= 8.61D-01
 SS=  1.41D+00  RLast= 8.46D-02 DXNew= 1.4142D-01 2.5393D-01
 Trust test= 8.61D-01 RLast= 8.46D-02 DXMaxT set to 1.41D-01
     Eigenvalues ---    0.00001   0.00079   0.01449   0.01567
0.01710
     Eigenvalues ---    0.01801   0.01816   0.01893   0.01942
0.01975
     Eigenvalues ---    0.01990   0.02018   0.02048   0.02078
0.02113
     Eigenvalues ---    0.02144   0.02170   0.02183   0.02228
0.02266
     Eigenvalues ---    0.02342   0.02554   0.04508   0.06746
0.07475
     Eigenvalues ---    0.11977   0.13536   0.15626   0.15946
0.15994
     Eigenvalues ---    0.15999   0.16001   0.16005   0.16018
0.16067
     Eigenvalues ---    0.16512   0.16595   0.21450   0.21980
0.22115
     Eigenvalues ---    0.22611   0.23190   0.23578   0.24395
0.24835
     Eigenvalues ---    0.25312   0.28745   0.31063   0.32393
0.33429
     Eigenvalues ---    0.33594   0.33631   0.33682   0.33683
0.33777
     Eigenvalues ---    0.33956   0.34212   0.34330   0.36158
0.37276
     Eigenvalues ---    0.38091   0.38379   0.38821   0.39616
0.40186
     Eigenvalues ---    0.41039   0.42190   0.43136   0.45170
0.46776
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.48802   0.49856   0.50941   0.51218
1.06521
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   1.30D-05 Eigenvector:
                          D46       D45       D43       D44       D42
   1                    0.40877   0.35292   0.33132   0.30912
0.27546
                          D41       R28       R16       R29       R27
   1                    0.23167  -0.18593   0.16362  -0.14599  -
0.14469
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    34   33
 RFO step:  Lambda=-3.99011087D-06.
 DIIS coeffs:      4.07968     -3.07968
 Maximum step size (   0.141) exceeded in Quadratic search.
    -- Step size scaled by   0.459
 Iteration  1 RMS(Cart)=  0.02795929 RMS(Int)=  0.00025040
 Iteration  2 RMS(Cart)=  0.00036431 RMS(Int)=  0.00003253
 Iteration  3 RMS(Cart)=  0.00000010 RMS(Int)=  0.00003253
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59048  -0.00001   0.00024  -0.01714  -0.01688
2.57360
```

This journal is © The Royal Society of Chemistry 2014

R2	2.69182	0.00001	0.00004	0.00392	0.00396
2.69578					
R3	2.05419	-0.00007	-0.00009	0.01060	0.01051
2.06469					
R4	2.70431	0.00003	-0.00007	0.00379	0.00374
2.70804					
R5	2.05609	-0.00006	-0.00006	0.01457	0.01451
2.07060					
R6	2.73148	0.00016	-0.00065	-0.02108	-0.02173
2.70976					
R7	2.64281	0.00000	0.00006	0.00406	0.00413
2.64694					
R8	2.71059	0.00019	-0.00020	0.02505	0.02484
2.73543					
R9	2.67904	0.00033	-0.00007	0.02475	0.02467
2.70372					
R10	2.59543	0.00000	0.00001	-0.00819	-0.00819
2.58724					
R11	2.04978	-0.00017	0.00002	0.00052	0.00054
2.05032					
R12	2.05460	-0.00006	-0.00004	0.00963	0.00960
2.06419					
R13	2.64141	-0.00005	-0.00025	-0.00372	-0.00396
2.63744					
R14	2.05719	-0.00006	-0.00006	0.01209	0.01203
2.06922					
R15	2.67866	-0.00015	0.00004	-0.00333	-0.00330
2.67536					
R16	2.86227	-0.00004	0.00048	0.03462	0.03510
2.89737					
R17	2.73916	0.00001	0.00082	-0.01622	-0.01539
2.72377					
R18	2.71413	-0.00006	0.00061	0.01934	0.01995
2.73408					
R19	2.70584	0.00003	0.00023	0.00728	0.00752
2.71336					
R20	2.05607	-0.00006	-0.00007	0.01445	0.01438
2.07045					
R21	2.58843	0.00007	-0.00015	-0.01686	-0.01701
2.57142					
R22	2.69226	0.00006	0.00010	0.00907	0.00916
2.70143					
R23	2.05414	-0.00007	-0.00011	0.01025	0.01014
2.06428					
R24	2.59375	0.00001	-0.00027	-0.01088	-0.01116
2.58259					
R25	2.05457	-0.00006	-0.00004	0.00947	0.00944
2.06400					
R26	2.04833	-0.00004	-0.00038	0.00557	0.00519
2.05352					
R27	2.07698	-0.00001	0.00009	-0.03147	-0.03139
2.04559					

This journal is © The Royal Society of Chemistry 2014

R28	2.06024	0.00015	-0.00060	-0.04015	-0.04076
2.01948					
R29	2.06931	0.00011	0.00104	-0.03106	-0.03002
2.03928					
A1	2.09046	0.00000	0.00017	0.00052	0.00069
2.09115					
A2	2.10194	-0.00001	-0.00012	0.01029	0.01017
2.11211					
A3	2.09077	0.00001	-0.00005	-0.01081	-0.01086
2.07991					
A4	2.11545	0.00002	-0.00009	0.00038	0.00031
2.11576					
A5	2.10436	-0.00002	-0.00010	0.01024	0.01012
2.11448					
A6	2.06336	0.00001	0.00019	-0.01059	-0.01042
2.05294					
A7	2.08400	0.00006	-0.00025	0.00895	0.00870
2.09270					
A8	2.11577	-0.00008	0.00073	-0.01153	-0.01083
2.10493					
A9	2.08342	0.00003	-0.00047	0.00260	0.00210
2.08552					
A10	2.04732	-0.00014	0.00063	-0.00952	-0.00888
2.03844					
A11	2.09739	-0.00012	0.00083	-0.00497	-0.00417
2.09322					
A12	2.13844	0.00026	-0.00145	0.01451	0.01308
2.15152					
A13	2.12254	0.00005	-0.00024	0.00041	0.00014
2.12268					
A14	2.08523	0.00004	-0.00062	-0.00595	-0.00656
2.07867					
A15	2.07531	-0.00010	0.00087	0.00559	0.00647
2.08178					
A16	2.10644	0.00002	-0.00020	-0.00072	-0.00094
2.10550					
A17	2.08604	-0.00001	0.00002	-0.01001	-0.00998
2.07606					
A18	2.09070	-0.00001	0.00018	0.01074	0.01092
2.10162					
A19	2.11889	0.00002	0.00001	-0.00048	-0.00048
2.11841					
A20	2.08256	-0.00001	0.00006	0.00134	0.00138
2.08394					
A21	2.08171	-0.00002	-0.00007	-0.00079	-0.00088
2.08083					
A22	2.08780	-0.00001	-0.00003	0.00016	0.00007
2.08787					
A23	2.07585	0.00043	-0.00413	-0.00322	-0.00735
2.06850					
A24	2.11951	-0.00042	0.00416	0.00298	0.00713
2.12664					

This journal is © The Royal Society of Chemistry 2014

```
   A25        2.08881   0.00008  -0.00075  -0.00176  -0.00254
2.08628
   A26        2.15393  -0.00014   0.00155   0.01031   0.01188
2.16581
   A27        2.04042   0.00005  -0.00080  -0.00853  -0.00932
2.03109
   A28        2.08906   0.00000   0.00052   0.00498   0.00549
2.09455
   A29        2.10833   0.00001  -0.00066  -0.01165  -0.01232
2.09601
   A30        2.08579  -0.00002   0.00015   0.00668   0.00684
2.09263
   A31        2.06142   0.00002  -0.00012  -0.01178  -0.01191
2.04951
   A32        2.11728  -0.00002   0.00026   0.00094   0.00121
2.11849
   A33        2.10448   0.00000  -0.00014   0.01085   0.01070
2.11518
   A34        2.08835   0.00000  -0.00022  -0.00115  -0.00137
2.08698
   A35        2.10320  -0.00001   0.00010   0.01111   0.01121
2.11441
   A36        2.09163   0.00001   0.00012  -0.00996  -0.00984
2.08178
   A37        2.10819  -0.00001   0.00011  -0.00041  -0.00033
2.10786
   A38        2.08602   0.00002  -0.00004  -0.00861  -0.00864
2.07738
   A39        2.08897  -0.00001  -0.00007   0.00903   0.00897
2.09795
   A40        2.12617  -0.00001   0.00050   0.00232   0.00280
2.12896
   A41        2.08959  -0.00001   0.00032  -0.00572  -0.00538
2.08421
   A42        2.06730   0.00002  -0.00083   0.00334   0.00253
2.06982
   A43        1.95034  -0.00010  -0.00053   0.00233   0.00172
1.95206
   A44        1.96519  -0.00001   0.00268   0.02063   0.02320
1.98839
   A45        1.93862   0.00011  -0.00228   0.00158  -0.00077
1.93785
   A46        1.87444  -0.00004   0.00052  -0.00643  -0.00601
1.86843
   A47        1.87094  -0.00002  -0.00079  -0.01899  -0.01981
1.85113
   A48        1.85902   0.00005   0.00037  -0.00132  -0.00105
1.85797
    D1       -0.00109   0.00000   0.00017  -0.00032  -0.00012  -
0.00121
    D2        3.13467   0.00004   0.00063   0.00411   0.00476
3.13943
```

This journal is © The Royal Society of Chemistry 2014

D3	-3.13861	-0.00002	-0.00032	-0.00184	-0.00215	-3.14076
D4	-0.00285	0.00002	0.00014	0.00259	0.00274	-0.00012
D5	0.01078	-0.00006	-0.00053	0.00267	0.00216	0.01294
D6	-3.12812	-0.00006	-0.00074	-0.00227	-0.00299	-3.13110
D7	-3.13486	-0.00003	-0.00004	0.00423	0.00420	-3.13066
D8	0.00943	-0.00004	-0.00025	-0.00071	-0.00095	0.00849
D9	-0.01383	0.00007	0.00068	0.00063	0.00128	-0.01255
D10	3.12548	0.00007	0.00123	0.01069	0.01187	3.13735
D11	3.13346	0.00003	0.00023	-0.00376	-0.00350	3.12996
D12	-0.01042	0.00003	0.00079	0.00630	0.00709	-0.00333
D13	0.01876	-0.00008	-0.00114	-0.00338	-0.00446	0.01429
D14	-3.13182	-0.00003	-0.00015	-0.00089	-0.00098	-3.13280
D15	-3.12059	-0.00008	-0.00168	-0.01323	-0.01492	-3.13551
D16	0.01202	-0.00003	-0.00069	-0.01074	-0.01144	0.00058
D17	-3.12092	-0.00009	-0.00191	-0.01230	-0.01409	-3.13501
D18	0.01309	-0.00008	-0.00097	-0.00145	-0.00232	0.01076
D19	0.01838	-0.00009	-0.00136	-0.00224	-0.00353	0.01485
D20	-3.13079	-0.00008	-0.00042	0.00862	0.00823	-3.12256
D21	-0.00956	0.00002	0.00080	0.00589	0.00667	-0.00289
D22	3.11612	0.00010	0.00133	0.00956	0.01089	3.12701
D23	3.14124	-0.00002	-0.00022	0.00345	0.00316	-3.13878
D24	-0.01626	0.00006	0.00031	0.00713	0.00738	-0.00888
D25	-0.04363	0.00017	0.00223	0.01552	0.01778	-0.02585
D26	3.10512	0.00019	0.00171	0.02860	0.03026	3.13538
D27	3.08849	0.00022	0.00329	0.01801	0.02137	3.10986
D28	-0.04594	0.00024	0.00276	0.03109	0.03385	-0.01209

This journal is © The Royal Society of Chemistry 2014

D29	-0.00516	0.00004	0.00002	-0.00556	-0.00556	-0.01073
D30	3.13372	0.00005	0.00023	-0.00064	-0.00038	3.13335
D31	-3.13094	-0.00004	-0.00049	-0.00912	-0.00967	-3.14061
D32	0.00795	-0.00003	-0.00029	-0.00420	-0.00449	0.00346
D33	-0.01664	0.00008	0.00182	0.00989	0.01175	-0.00489
D34	3.12207	0.00007	0.00189	0.01390	0.01578	3.13784
D35	3.13253	0.00006	0.00088	-0.00097	0.00000	3.13253
D36	-0.01195	0.00005	0.00095	0.00304	0.00403	-0.00792
D37	0.04521	-0.00018	-0.00180	-0.00775	-0.00955	0.03565
D38	-3.08844	-0.00017	-0.00225	-0.01052	-0.01280	-3.10124
D39	-3.10373	-0.00020	-0.00130	-0.02119	-0.02253	-3.12626
D40	0.04580	-0.00019	-0.00175	-0.02396	-0.02577	0.02003
D41	1.30240	-0.00002	-0.05008	0.02695	-0.02314	1.27926
D42	-2.86934	-0.00014	-0.04788	0.03504	-0.01282	-2.88216
D43	-0.78605	0.00000	-0.04717	0.04840	0.00127	-0.78478
D44	-1.83189	0.00001	-0.05059	0.04029	-0.01034	-1.84223
D45	0.27955	-0.00012	-0.04839	0.04838	-0.00002	0.27954
D46	2.36284	0.00002	-0.04768	0.06174	0.01407	2.37691
D47	-0.01551	0.00006	-0.00023	-0.00497	-0.00519	-0.02069
D48	3.12894	0.00007	-0.00029	-0.00889	-0.00917	3.11977
D49	3.11865	0.00005	0.00021	-0.00229	-0.00209	3.11656
D50	-0.02009	0.00005	0.00015	-0.00622	-0.00608	-0.02617
D51	-3.13862	-0.00001	0.00046	0.00292	0.00339	-3.13523
D52	0.02027	-0.00009	0.00056	0.00650	0.00705	0.02732
D53	0.01071	0.00000	0.00001	0.00019	0.00021	0.01092
D54	-3.11359	-0.00007	0.00012	0.00377	0.00388	-3.10971

```
   D55        0.01138  -0.00002   0.00003   0.00355   0.00362
0.01500
   D56       -3.12416  -0.00005  -0.00020   0.00156   0.00142  -
3.12273
   D57       -3.13310  -0.00003   0.00010   0.00755   0.00764  -
3.12546
   D58        0.01455  -0.00006  -0.00013   0.00556   0.00544
0.01999
   D59        0.00133   0.00001  -0.00003   0.00148   0.00148
0.00281
   D60        3.13874   0.00001   0.00007   0.00025   0.00032
3.13906
   D61       -3.13405  -0.00003  -0.00027  -0.00048  -0.00073  -
3.13478
   D62        0.00336  -0.00002  -0.00017  -0.00171  -0.00188
0.00147
   D63       -0.01127   0.00005   0.00020  -0.00762  -0.00742  -
0.01870
   D64        3.12692   0.00005   0.00022  -0.00453  -0.00433
3.12259
   D65        3.13448   0.00004   0.00009  -0.00644  -0.00634
3.12814
   D66       -0.01051   0.00005   0.00012  -0.00335  -0.00325  -
0.01376
   D67        0.00490  -0.00005  -0.00019   0.00673   0.00653
0.01143
   D68        3.12941   0.00002  -0.00028   0.00310   0.00282
3.13222
   D69       -3.13329  -0.00006  -0.00021   0.00367   0.00343  -
3.12985
   D70       -0.00878   0.00001  -0.00030   0.00004  -0.00028  -
0.00906
         Item               Value     Threshold  Converged?
 Maximum Force            0.000432     0.000450     YES
 RMS     Force            0.000096     0.000300     YES
 Maximum Displacement     0.093343     0.001800     NO
 RMS     Displacement     0.027982     0.001200     NO
 Predicted change in Energy=-2.385391D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.780348   -5.430866    0.017883
      2          6           0       -3.419205   -5.388245    0.003119
      3          6           0       -2.715147   -4.140157   -0.009647
      4          6           0       -3.446599   -2.906867   -0.022564
      5          6           0       -4.890707   -3.004471   -0.003391
```

This journal is © The Royal Society of Chemistry 2014

6	6	0	-5.527996	-4.215944	0.022308
7	6	0	-1.314778	-4.111456	-0.019657
8	6	0	-2.744344	-1.660549	-0.046211
9	6	0	-1.328778	-1.654342	-0.024889
10	6	0	-0.612695	-2.905235	-0.024305
11	6	0	0.823139	-2.907984	-0.029922
12	1	0	1.325911	-3.881333	-0.044940
13	6	0	1.533997	-1.747815	-0.012625
14	6	0	0.842478	-0.496977	0.015173
15	6	0	-0.523394	-0.452733	0.002617
16	1	0	-0.757845	-5.054190	-0.027924
17	1	0	-5.313660	-6.384395	0.028367
18	1	0	-2.823315	-6.307760	0.001471
19	1	0	-5.481064	-2.094175	0.001512
20	1	0	-6.618928	-4.266541	0.044218
21	1	0	2.626344	-1.754403	-0.014605
22	1	0	1.421938	0.428315	0.047041
23	1	0	-1.012612	0.517098	0.033585
24	6	0	-3.558829	-0.361739	-0.067857
25	1	0	-4.015603	-0.156709	0.891874
26	1	0	-2.989652	0.502372	-0.335044
27	1	0	-4.369738	-0.424913	-0.777070

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.361889	0.000000			
3	C	2.435517	1.433034	0.000000		
4	C	2.855011	2.481662	1.433943	0.000000	
5	C	2.428996	2.801382	2.454156	1.447530	0.000000
6	C	1.426546	2.412811	2.814051	2.459249	1.369111
7	C	3.708426	2.461570	1.400699	2.448613	3.743388
8	C	4.285406	3.788613	2.480049	1.430744	2.532752
9	C	5.116375	4.279335	2.846318	2.460486	3.809285
10	C	4.873389	3.747345	2.438350	2.833905	4.279214
11	C	6.145428	4.914293	3.746749	4.269745	5.714722
12	H	6.300111	4.978878	4.049493	4.871031	6.278293
13	C	7.310044	6.147129	4.876324	5.113691	6.546456
14	C	7.480604	6.487419	5.092158	4.919876	6.257579
15	C	6.550091	5.722325	4.289642	3.816875	5.058145
16	H	4.040360	2.682423	2.160283	3.440992	4.613296
17	H	1.092589	2.140540	3.433703	3.947367	3.406433
18	H	2.144572	1.095717	2.170329	3.457619	3.896903
19	H	3.409513	3.886150	3.440416	2.190912	1.084981
20	H	2.176401	3.390890	3.906197	3.452078	2.140522
21	H	8.269009	7.053637	5.850075	6.181333	7.620292
22	H	8.532244	7.567758	6.163572	5.901774	7.185823
23	H	7.040906	6.376966	4.958883	4.201308	5.238553
24	C	5.214931	5.028946	3.871903	2.548004	2.960083
25	H	5.400502	5.339901	4.286231	2.953529	3.110796
26	H	6.207614	5.915932	4.662007	3.453891	4.002744
27	H	5.085284	5.113402	4.138798	2.753464	2.743011

		6	7	8	9	10
6	C	0.000000				
7	C	4.214722	0.000000			
8	C	3.779345	2.837483	0.000000		
9	C	4.919091	2.457159	1.415741	0.000000	
10	C	5.087269	1.395676	2.468532	1.441356	0.000000
11	C	6.484628	2.453393	3.779325	2.490460	1.435848
12	H	6.862400	2.650818	4.636686	3.465150	2.170573
13	C	7.480950	3.701671	4.279363	2.864326	2.438861
14	C	7.376565	4.209445	3.771335	2.460783	2.814036
15	C	6.261644	3.743400	2.528601	1.446812	2.454275
16	H	4.843503	1.094984	3.932342	3.447454	2.153855
17	H	2.179026	4.599958	5.377886	6.185105	5.848624
18	H	3.419272	2.664560	4.648126	4.887600	4.057669
19	H	2.122390	4.629019	2.771272	4.175600	4.935535
20	H	1.092325	5.306801	4.670307	5.900343	6.158951
21	H	8.517852	4.592185	5.371601	3.956401	3.437424
22	H	8.358907	5.301281	4.661540	3.450952	3.906069
23	H	6.541445	4.638713	2.783417	2.195116	3.446107
24	C	4.329047	4.370180	1.533220	2.577945	3.892426
25	H	4.418242	4.874974	2.181201	3.209733	4.469179
26	H	5.369674	4.918545	2.195867	2.739729	4.166326
27	H	4.043821	4.847376	2.168607	3.365221	4.564430

		11	12	13	14	15
11	C	0.000000				
12	H	1.095634	0.000000			
13	C	1.360739	2.143885	0.000000		
14	C	2.411507	3.419238	1.429534	0.000000	
15	C	2.800441	3.895830	2.431117	1.366647	0.000000
16	H	2.665655	2.391218	4.023045	4.830227	4.607528
17	H	7.053306	7.096098	8.269822	8.518210	7.624430
18	H	4.985588	4.806848	6.307096	6.870476	6.290547
19	H	6.356591	7.037827	7.023621	6.522149	5.222339
20	H	7.565417	7.954672	8.533311	8.359608	7.190438
21	H	2.140685	2.493166	1.092369	2.182701	3.408151
22	H	3.390483	4.311698	2.179830	1.092224	2.136009
23	H	3.886541	4.982073	3.408399	2.114249	1.086676
24	C	5.068180	6.020694	5.278365	4.404167	3.037616
25	H	5.642043	6.578922	5.843611	4.948266	3.615789
26	H	5.124549	6.158337	5.062676	3.975748	2.666208
27	H	5.804295	6.702483	6.098240	5.272574	3.924671

		16	17	18	19	20
16	H	0.000000				
17	H	4.746374	0.000000			
18	H	2.416292	2.491669	0.000000		
19	H	5.574169	4.293569	4.981759	0.000000	
20	H	5.914211	2.487826	4.309881	2.452699	0.000000
21	H	4.726681	9.191427	7.101557	8.114541	9.580676
22	H	5.900418	9.580273	7.962346	7.349589	9.311133
23	H	5.577450	8.132014	7.061046	5.175601	7.369810
24	C	5.464998	6.273841	5.991741	2.588655	4.962283
25	H	5.953515	6.419865	6.328491	2.587295	4.938273

This journal is © The Royal Society of Chemistry 2014

```
   26  H    5.995888   7.277407   6.820470   3.614203   6.004834
   27  H    5.919223   6.087294   6.132328   2.151203   4.526752
                 21         22         23         24         25
   21  H    0.000000
   22  H    2.493723   0.000000
   23  H    4.289993   2.436205   0.000000
   24  C    6.340246   5.044346   2.695527   0.000000
   25  H    6.891284   5.533791   3.195095   1.082480   0.000000
   26  H    6.060951   4.428724   2.011166   1.068663   1.729825
   27  H    7.161987   5.911908   3.579782   1.079141   1.727055
                 26         27
   26  H    0.000000
   27  H    1.720431   0.000000
Stoichiometry    C15H12
Framework group  C1[X(C15H12)]
Deg. of freedom    75
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -3.647969   -1.020670    0.016174
     2          6           0       -2.449193   -1.666766    0.000647
     3          6           0       -1.213864   -0.940462   -0.004851
     4          6           0       -1.227638    0.493407   -0.009508
     5          6           0       -2.525779    1.133553    0.010146
     6          6           0       -3.685012    0.405339    0.028756
     7          6           0        0.011845   -1.618310   -0.015741
     8          6           0        0.005270    1.219147   -0.025898
     9          6           0        1.232758    0.514036   -0.005608
    10          6           0        1.224436   -0.927275   -0.013382
    11          6           0        2.465027   -1.650148   -0.020101
    12          1           0        2.411511   -2.744263   -0.041582
    13          6           0        3.662045   -1.003476    0.003907
    14          6           0        3.691517    0.425297    0.040044
    15          6           0        2.532308    1.149058    0.028797
    16          1           0        0.020521   -2.713162   -0.030320
    17          1           0       -4.587788   -1.577864    0.021103
    18          1           0       -2.395184   -2.761122   -0.007197
    19          1           0       -2.579636    2.217141    0.021184
    20          1           0       -4.654084    0.908897    0.051175
    21          1           0        4.603594   -1.557323    0.001060
    22          1           0        4.656977    0.934664    0.077255
    23          1           0        2.595744    2.233236    0.066195
    24          6           0       -0.047424    2.751407   -0.038812
    25          1           0       -0.342017    3.152414    0.922527
    26          1           0        0.879184    3.214746   -0.301024
    27          1           0       -0.778780    3.107796   -0.747792
---------------------------------------------------------------------
```

```
 Rotational constants (GHZ):      1.3878404      0.4464306
0.3385058
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       877.8665415738 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
```

```
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.858721271     A.U. after   13 cycles
            Convg  =    0.4197D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.009881368   -0.003451131    0.000409720
      2        6           0.010085531   -0.003438469   -0.000072995
      3        6           0.005172314   -0.005763028   -0.000661203
      4        6          -0.005537379    0.009386791   -0.000129570
      5        6           0.008533433    0.006371653    0.000303949
      6        6          -0.003540732   -0.003332825   -0.000307338
      7        6           0.000457192   -0.003382084   -0.000539102
      8        6          -0.009710747    0.002091496    0.001134673
      9        6           0.001147421    0.006585058   -0.000318627
     10        6           0.004102238   -0.005092898   -0.000299507
     11        6          -0.002290914   -0.009978375   -0.000013574
     12        1          -0.001465936    0.004935332    0.000170122
     13        6           0.006633747    0.007399149    0.000318854
     14        6           0.005994259    0.000511339   -0.000297175
     15        6          -0.009515129   -0.000378199    0.000631628
     16        1          -0.002409318    0.003646350    0.000388475
     17        1           0.002596006    0.002773828    0.000035087
     18        1          -0.003523969    0.003807023    0.000083303
     19        1          -0.000210030   -0.000346900    0.000135156
     20        1           0.003433387    0.001349378   -0.000211657
     21        1          -0.003624473   -0.000849658    0.000049151
     22        1          -0.002598574   -0.002430623   -0.000276440
     23        1           0.000222027   -0.001382186   -0.000381733
     24        6           0.005205983   -0.019138020    0.001588039
     25        1          -0.003133326    0.000680268    0.010931683
     26        1           0.011208342    0.011059799   -0.004142683
     27        1          -0.007349986   -0.001633067   -0.008528237
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.019138020 RMS     0.005116127
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.015947150 RMS     0.002966855
 Search for a local minimum.
 Step number  35 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points   13   14   15   16
17
                                                     18   19   21   20
23
                                                     22   25   24   27
26
                                                     28   29   30   31
32
                                                     33   35   34
 DE=  1.89D-03 DEPred=-2.39D-05 R=-7.93D+01
 Trust test=-7.93D+01 RLast= 1.41D-01 DXMaxT set to 7.07D-02
 Use linear search instead of GDIIS.
 Quartic linear search produced a step of -0.99210.
 Iteration  1 RMS(Cart)=  0.02774525 RMS(Int)=  0.00024202
 Iteration  2 RMS(Cart)=  0.00035804 RMS(Int)=  0.00000027
 Iteration  3 RMS(Cart)=  0.00000009 RMS(Int)=  0.00000026
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.57360   0.00694   0.01675   0.00000   0.01675
2.59035
    R2        2.69578   0.00045  -0.00393   0.00000  -0.00393
2.69185
    R3        2.06469  -0.00369  -0.01042   0.00000  -0.01042
2.05427
    R4        2.70804  -0.00018  -0.00371   0.00000  -0.00371
2.70434
    R5        2.07060  -0.00511  -0.01440   0.00000  -0.01440
2.05621
    R6        2.70976   0.00651   0.02155   0.00000   0.02155
2.73131
    R7        2.64694  -0.00033  -0.00410   0.00000  -0.00410
2.64284
    R8        2.73543  -0.00808  -0.02464   0.00000  -0.02464
2.71079
    R9        2.70372  -0.01010  -0.02448   0.00000  -0.02448
2.67924
   R10        2.58724   0.00261   0.00813   0.00000   0.00813
2.59537
   R11        2.05032  -0.00018  -0.00053   0.00000  -0.00053
2.04978
```

This journal is © The Royal Society of Chemistry 2014

R12	2.06419	-0.00350	-0.00952	0.00000	-0.00952
2.05467					
R13	2.63744	0.00093	0.00393	0.00000	0.00393
2.64137					
R14	2.06922	-0.00437	-0.01194	0.00000	-0.01194
2.05728					
R15	2.67536	-0.00303	0.00328	0.00000	0.00328
2.67864					
R16	2.89737	-0.01080	-0.03482	0.00000	-0.03482
2.86254					
R17	2.72377	0.00459	0.01527	0.00000	0.01527
2.73904					
R18	2.73408	-0.00592	-0.01979	0.00000	-0.01979
2.71428					
R19	2.71336	-0.00071	-0.00746	0.00000	-0.00746
2.70590					
R20	2.07045	-0.00506	-0.01427	0.00000	-0.01427
2.05618					
R21	2.57142	0.00672	0.01687	0.00000	0.01687
2.58830					
R22	2.70143	-0.00050	-0.00909	0.00000	-0.00909
2.69234					
R23	2.06428	-0.00362	-0.01006	0.00000	-0.01006
2.05422					
R24	2.58259	0.00339	0.01108	0.00000	0.01108
2.59366					
R25	2.06400	-0.00345	-0.00936	0.00000	-0.00936
2.05464					
R26	2.05352	-0.00134	-0.00515	0.00000	-0.00515
2.04837					
R27	2.04559	0.01115	0.03114	0.00000	0.03114
2.07673					
R28	2.01948	0.01595	0.04043	0.00000	0.04043
2.05991					
R29	2.03928	0.01122	0.02979	0.00000	0.02979
2.06907					
A1	2.09115	-0.00064	-0.00069	0.00000	-0.00069
2.09047					
A2	2.11211	-0.00062	-0.01009	0.00000	-0.01009
2.10202					
A3	2.07991	0.00126	0.01077	0.00000	0.01077
2.09069					
A4	2.11576	-0.00110	-0.00031	0.00000	-0.00031
2.11545					
A5	2.11448	-0.00037	-0.01004	0.00000	-0.01004
2.10444					
A6	2.05294	0.00147	0.01034	0.00000	0.01034
2.06328					
A7	2.09270	-0.00184	-0.00864	0.00000	-0.00864
2.08407					
A8	2.10493	0.00219	0.01075	0.00000	0.01075
2.11568					

This journal is © The Royal Society of Chemistry 2014

A9	2.08552	-0.00035	-0.00208	0.00000	-0.00208
2.08343					
A10	2.03844	0.00299	0.00881	0.00000	0.00881
2.04725					
A11	2.09322	0.00091	0.00414	0.00000	0.00414
2.09736					
A12	2.15152	-0.00390	-0.01297	0.00000	-0.01297
2.13854					
A13	2.12268	-0.00018	-0.00014	0.00000	-0.00014
2.12254					
A14	2.07867	0.00047	0.00651	0.00000	0.00651
2.08518					
A15	2.08178	-0.00029	-0.00642	0.00000	-0.00642
2.07536					
A16	2.10550	0.00077	0.00094	0.00000	0.00094
2.10643					
A17	2.07606	0.00084	0.00990	0.00000	0.00990
2.08596					
A18	2.10162	-0.00161	-0.01084	0.00000	-0.01084
2.09079					
A19	2.11841	-0.00113	0.00047	0.00000	0.00047
2.11889					
A20	2.08394	0.00033	-0.00136	0.00000	-0.00136
2.08257					
A21	2.08083	0.00079	0.00088	0.00000	0.00088
2.08170					
A22	2.08787	0.00101	-0.00007	0.00000	-0.00007
2.08781					
A23	2.06850	0.00190	0.00729	0.00000	0.00729
2.07579					
A24	2.12664	-0.00291	-0.00708	0.00000	-0.00708
2.11956					
A25	2.08628	0.00143	0.00252	0.00000	0.00252
2.08879					
A26	2.16581	-0.00464	-0.01178	0.00000	-0.01178
2.15402					
A27	2.03109	0.00321	0.00925	0.00000	0.00925
2.04034					
A28	2.09455	-0.00187	-0.00544	0.00000	-0.00544
2.08911					
A29	2.09601	0.00353	0.01223	0.00000	0.01223
2.10823					
A30	2.09263	-0.00165	-0.00678	0.00000	-0.00678
2.08584					
A31	2.04951	0.00151	0.01181	0.00000	0.01181
2.06132					
A32	2.11849	-0.00103	-0.00120	0.00000	-0.00120
2.11729					
A33	2.11518	-0.00048	-0.01062	0.00000	-0.01062
2.10456					
A34	2.08698	-0.00004	0.00136	0.00000	0.00136
2.08834					

A35	2.11441	-0.00088	-0.01112	0.00000	-0.01112
2.10328					
A36	2.08178	0.00092	0.00977	0.00000	0.00977
2.09155					
A37	2.10786	0.00040	0.00033	0.00000	0.00033
2.10818					
A38	2.07738	0.00074	0.00857	0.00000	0.00857
2.08595					
A39	2.09795	-0.00114	-0.00890	0.00000	-0.00890
2.08905					
A40	2.12896	-0.00088	-0.00278	0.00000	-0.00278
2.12619					
A41	2.08421	0.00000	0.00534	0.00000	0.00534
2.08955					
A42	2.06982	0.00088	-0.00251	0.00000	-0.00251
2.06732					
A43	1.95206	-0.00179	-0.00171	0.00000	-0.00171
1.95035					
A44	1.98839	-0.00407	-0.02302	0.00000	-0.02301
1.96538					
A45	1.93785	-0.00054	0.00076	0.00000	0.00076
1.93861					
A46	1.86843	0.00252	0.00596	0.00000	0.00596
1.87440					
A47	1.85113	0.00250	0.01965	0.00000	0.01965
1.87079					
A48	1.85797	0.00208	0.00104	0.00000	0.00104
1.85901					
D1	-0.00121	0.00002	0.00012	0.00000	0.00012	-
0.00109					
D2	3.13943	0.00000	-0.00472	0.00000	-0.00472
3.13471					
D3	-3.14076	-0.00002	0.00213	0.00000	0.00213	-
3.13863					
D4	-0.00012	-0.00003	-0.00271	0.00000	-0.00271	-
0.00283					
D5	0.01294	-0.00018	-0.00214	0.00000	-0.00214
0.01080					
D6	-3.13110	-0.00007	0.00296	0.00000	0.00296	-
3.12814					
D7	-3.13066	-0.00015	-0.00416	0.00000	-0.00416	-
3.13482					
D8	0.00849	-0.00003	0.00094	0.00000	0.00094
0.00943					
D9	-0.01255	0.00014	-0.00127	0.00000	-0.00127	-
0.01382					
D10	3.13735	-0.00009	-0.01178	0.00000	-0.01178
3.12557					
D11	3.12996	0.00016	0.00347	0.00000	0.00347
3.13343					
D12	-0.00333	-0.00008	-0.00704	0.00000	-0.00704	-
0.01036					

This journal is © The Royal Society of Chemistry 2014

D13	0.01429	-0.00007	0.00443	0.00000	0.00443	0.01872
D14	-3.13280	-0.00014	0.00097	0.00000	0.00097	-3.13183
D15	-3.13551	0.00018	0.01480	0.00000	0.01480	-3.12071
D16	0.00058	0.00010	0.01135	0.00000	0.01135	0.01193
D17	-3.13501	0.00011	0.01398	0.00000	0.01398	-3.12104
D18	0.01076	-0.00008	0.00231	0.00000	0.00231	0.01307
D19	0.01485	-0.00012	0.00350	0.00000	0.00350	0.01835
D20	-3.12256	-0.00031	-0.00817	0.00000	-0.00817	-3.13073
D21	-0.00289	-0.00011	-0.00662	0.00000	-0.00662	-0.00951
D22	3.12701	-0.00005	-0.01080	0.00000	-0.01080	3.11621
D23	-3.13878	-0.00005	-0.00314	0.00000	-0.00314	3.14127
D24	-0.00888	0.00001	-0.00732	0.00000	-0.00732	-0.01620
D25	-0.02585	0.00001	-0.01764	0.00000	-0.01764	-0.04349
D26	3.13538	-0.00009	-0.03002	0.00000	-0.03002	3.10536
D27	3.10986	-0.00004	-0.02120	0.00000	-0.02120	3.08866
D28	-0.01209	-0.00014	-0.03359	0.00000	-0.03359	-0.04567
D29	-0.01073	0.00022	0.00552	0.00000	0.00552	-0.00521
D30	3.13335	0.00010	0.00037	0.00000	0.00037	3.13372
D31	-3.14061	0.00016	0.00960	0.00000	0.00960	-3.13101
D32	0.00346	0.00004	0.00445	0.00000	0.00445	0.00792
D33	-0.00489	-0.00002	-0.01166	0.00000	-0.01166	-0.01655
D34	3.13784	-0.00009	-0.01565	0.00000	-0.01565	3.12219
D35	3.13253	0.00016	0.00000	0.00000	0.00000	3.13253
D36	-0.00792	0.00009	-0.00399	0.00000	-0.00399	-0.01192
D37	0.03565	-0.00012	0.00948	0.00000	0.00948	0.04513
D38	-3.10124	-0.00013	0.01270	0.00000	0.01270	-3.08855

This journal is © The Royal Society of Chemistry 2014

D39	-3.12626	0.00004	0.02235	0.00000	0.02235	-3.10391
D40	0.02003	0.00003	0.02557	0.00000	0.02557	0.04560
D41	1.27926	0.00083	0.02296	0.00000	0.02296	1.30222
D42	-2.88216	-0.00023	0.01272	0.00000	0.01272	-2.86944
D43	-0.78478	-0.00079	-0.00126	0.00000	-0.00126	-0.78604
D44	-1.84223	0.00067	0.01025	0.00000	0.01025	-1.83198
D45	0.27954	-0.00039	0.00002	0.00000	0.00002	0.27955
D46	2.37691	-0.00095	-0.01396	0.00000	-0.01396	2.36295
D47	-0.02069	0.00017	0.00515	0.00000	0.00515	-0.01555
D48	3.11977	0.00024	0.00910	0.00000	0.00910	3.12886
D49	3.11656	0.00015	0.00208	0.00000	0.00208	3.11864
D50	-0.02617	0.00023	0.00603	0.00000	0.00603	-0.02014
D51	-3.13523	0.00000	-0.00336	0.00000	-0.00336	-3.13860
D52	0.02732	-0.00025	-0.00700	0.00000	-0.00700	0.02032
D53	0.01092	-0.00001	-0.00021	0.00000	-0.00021	0.01071
D54	-3.10971	-0.00025	-0.00385	0.00000	-0.00385	-3.11356
D55	0.01500	-0.00011	-0.00359	0.00000	-0.00359	0.01140
D56	-3.12273	-0.00018	-0.00141	0.00000	-0.00141	-3.12415
D57	-3.12546	-0.00018	-0.00758	0.00000	-0.00758	-3.13304
D58	0.01999	-0.00025	-0.00540	0.00000	-0.00540	0.01460
D59	0.00281	-0.00005	-0.00146	0.00000	-0.00146	0.00135
D60	3.13906	0.00008	-0.00031	0.00000	-0.00031	3.13874
D61	-3.13478	-0.00012	0.00072	0.00000	0.00072	-3.13406
D62	0.00147	0.00001	0.00187	0.00000	0.00187	0.00334
D63	-0.01870	0.00025	0.00737	0.00000	0.00737	-0.01133
D64	3.12259	0.00019	0.00430	0.00000	0.00430	3.12689

```
   D65        3.12814   0.00013   0.00629   0.00000   0.00629
3.13443
   D66       -0.01376   0.00006   0.00322   0.00000   0.00322  -
0.01054
   D67        0.01143  -0.00022  -0.00648   0.00000  -0.00648
0.00495
   D68        3.13222   0.00001  -0.00279   0.00000  -0.00279
3.12943
   D69       -3.12985  -0.00015  -0.00341   0.00000  -0.00341  -
3.13326
   D70       -0.00906   0.00008   0.00028   0.00000   0.00028  -
0.00878
         Item               Value     Threshold  Converged?
 Maximum Force            0.015947     0.000450     NO
 RMS     Force            0.002967     0.000300     NO
 Maximum Displacement     0.092602     0.001800     NO
 RMS     Displacement     0.027761     0.001200     NO
 Predicted change in Energy=-4.022633D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793031   -5.421340    0.021577
      2          6           0       -3.423004   -5.393551   -0.013303
      3          6           0       -2.706640   -4.154770   -0.027965
      4          6           0       -3.441236   -2.910031   -0.022988
      5          6           0       -4.872768   -2.991108    0.020601
      6          6           0       -5.524969   -4.199531    0.045169
      7          6           0       -1.308500   -4.126075   -0.044390
      8          6           0       -2.748100   -1.673502   -0.049294
      9          6           0       -1.330834   -1.664135   -0.026917
     10          6           0       -0.604648   -2.918512   -0.034224
     11          6           0        0.827170   -2.904638   -0.027416
     12          1           0        1.349101   -3.859269   -0.041332
     13          6           0        1.527468   -1.727928    0.002974
     14          6           0        0.823812   -0.489392    0.030100
     15          6           0       -0.548279   -0.460351    0.012802
     16          1           0       -0.756117   -5.064090   -0.058439
     17          1           0       -5.324445   -6.369570    0.035147
     18          1           0       -2.850756   -6.318943   -0.025179
     19          1           0       -5.458340   -2.078510    0.049626
     20          1           0       -6.611171   -4.226474    0.085535
     21          1           0        2.614477   -1.732671    0.010458
     22          1           0        1.381822    0.442990    0.068106
     23          1           0       -1.044838    0.502598    0.046157
     24          6           0       -3.546225   -0.386712   -0.091332
     25          1           0       -4.000456   -0.157305    0.882710
```

26	1	0	-2.940649	0.472786	-0.379033
27	1	0	-4.360274	-0.451981	-0.820632

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370753	0.000000			
3	C	2.441246	1.431073	0.000000		
4	C	2.852369	2.483606	1.445349	0.000000	
5	C	2.431540	2.806189	2.459386	1.434488	0.000000
6	C	1.424467	2.418132	2.819634	2.451408	1.373411
7	C	3.718066	2.465479	1.398530	2.455154	3.741173
8	C	4.270018	3.780946	2.481707	1.417791	2.501036
9	C	5.109379	4.276202	2.845366	2.450728	3.782646
10	C	4.879529	3.750917	2.438594	2.836622	4.269089
11	C	6.158153	4.925329	3.748418	4.268411	5.700795
12	H	6.337966	5.012763	4.066514	4.883515	6.282451
13	C	7.320543	6.159888	4.880388	5.107451	6.523722
14	C	7.474832	6.487534	5.089446	4.904380	6.221712
15	C	6.529120	5.709745	4.278892	3.790964	5.010588
16	H	4.053481	2.687540	2.152285	3.442542	4.609807
17	H	1.087072	2.137859	3.429610	3.939324	3.408553
18	H	2.140165	1.088098	2.168967	3.459675	3.894240
19	H	3.408510	3.890508	3.448004	2.182982	1.084699
20	H	2.176563	3.396505	3.906839	3.434136	2.133634
21	H	8.275118	7.060721	5.846566	6.169194	7.592273
22	H	8.515946	7.560304	6.153385	5.874771	7.135487
23	H	7.010178	6.357970	4.945519	4.170556	5.182632
24	C	5.187943	5.008963	3.860982	2.526427	2.924914
25	H	5.392568	5.343647	4.299189	2.951359	3.087815
26	H	6.191327	5.897485	4.646750	3.438140	3.986396
27	H	5.058767	5.094053	4.132007	2.742787	2.723507

		6	7	8	9	10
6	C	0.000000				
7	C	4.218060	0.000000			
8	C	3.755096	2.843869	0.000000		
9	C	4.901449	2.462104	1.417474	0.000000	
10	C	5.084965	1.397755	2.478843	1.449435	0.000000
11	C	6.483185	2.460342	3.781366	2.489142	1.431902
12	H	6.883031	2.670963	4.643781	3.464228	2.168459
13	C	7.473117	3.714306	4.276234	2.859170	2.442293
14	C	7.353393	4.216369	3.763905	2.454745	2.818734
15	C	6.224947	3.744161	2.512928	1.436337	2.459257
16	H	4.847696	1.088667	3.932451	3.448331	2.151054
17	H	2.179307	4.600805	5.357027	6.172026	5.847315
18	H	3.412956	2.680968	4.646637	4.896673	4.075293
19	H	2.122073	4.628448	2.742118	4.148960	4.926556
20	H	1.087285	5.305212	4.632404	5.870280	6.148449
21	H	8.505128	4.595775	5.363237	3.946084	3.430887
22	H	8.322097	5.303475	4.642152	3.436205	3.905923
23	H	6.494736	4.637061	2.765072	2.186747	3.450250
24	C	4.297866	4.358033	1.514793	2.558108	3.881514

This journal is © The Royal Society of Chemistry 2014

25	H	4.400592	4.884392	2.176208	3.197630	4.471750
26	H	5.356231	4.891362	2.179989	2.698503	4.132396
27	H	4.018739	4.838889	2.164759	3.358096	4.561463

		11	12	13	14	15
11	C	0.000000				
12	H	1.088084	0.000000			
13	C	1.369667	2.139251	0.000000		
14	C	2.415932	3.411320	1.424723	0.000000	
15	C	2.804998	3.893023	2.432195	1.372508	0.000000
16	H	2.677871	2.425660	4.043329	4.840648	4.608979
17	H	7.060597	7.130475	8.276146	8.507502	7.598101
18	H	5.018428	4.867141	6.344057	6.891238	6.294914
19	H	6.340035	7.037090	6.994754	6.480055	5.169960
20	H	7.555721	7.969747	8.513930	8.321528	7.137761
21	H	2.137618	2.475132	1.087046	2.180048	3.409081
22	H	3.394610	4.303776	2.176773	1.087270	2.131754
23	H	3.888327	4.976393	3.404977	2.115694	1.083953
24	C	5.046842	6.002114	5.248820	4.372930	3.000658
25	H	5.628689	6.570857	5.813668	4.910274	3.572968
26	H	5.072187	6.105956	4.995311	3.906961	2.597636
27	H	5.792606	6.694318	6.080450	5.253560	3.902049

		16	17	18	19	20
16	H	0.000000				
17	H	4.752122	0.000000			
18	H	2.441982	2.474942	0.000000		
19	H	5.571021	4.293174	4.978590	0.000000	
20	H	5.916417	2.500213	4.304811	2.438045	0.000000
21	H	4.739621	9.193908	7.134700	8.080316	9.557054
22	H	5.908869	9.559607	7.977917	7.290138	9.257005
23	H	5.575152	8.095792	7.056901	5.112839	7.304090
24	C	5.446435	6.242809	5.973225	2.556996	4.916193
25	H	5.957184	6.408085	6.333392	2.551564	4.899945
26	H	5.960869	7.257539	6.801534	3.609934	5.980937
27	H	5.902749	6.056389	6.110043	2.146787	4.487146

		21	22	23	24	25
21	H	0.000000				
22	H	2.501253	0.000000			
23	H	4.288157	2.427491	0.000000		
24	C	6.306839	4.999947	2.658328	0.000000	
25	H	6.855651	5.476573	3.141810	1.098959	0.000000
26	H	5.989588	4.345638	1.943134	1.090060	1.764143
27	H	7.139890	5.878987	3.557338	1.094904	1.765694

		26	27
26	H	0.000000	
27	H	1.750868	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

This journal is © The Royal Society of Chemistry 2014

```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.653825   -1.001648    0.023087
      2          6           0       -2.455318   -1.665972   -0.011805
      3          6           0       -1.213423   -0.954928   -0.020931
      4          6           0       -1.223014    0.490349   -0.010244
      5          6           0       -2.501493    1.139477    0.033121
      6          6           0       -3.672682    0.422395    0.052283
      7          6           0        0.009804   -1.632669   -0.037367
      8          6           0       -0.002307    1.211166   -0.031022
      9          6           0        1.227658    0.506949   -0.008745
     10          6           0        1.225139   -0.942425   -0.021804
     11          6           0        2.469984   -1.649996   -0.015078
     12          1           0        2.441522   -2.737554   -0.033367
     13          6           0        3.666698   -0.984720    0.020569
     14          6           0        3.680691    0.439557    0.053373
     15          6           0        2.509072    1.154258    0.036344
     16          1           0        0.016020   -2.721164   -0.055717
     17          1           0       -4.589807   -1.554438    0.032418
     18          1           0       -2.425589   -2.753545   -0.027928
     19          1           0       -2.549208    2.222617    0.066337
     20          1           0       -4.625393    0.944796    0.092636
     21          1           0        4.604079   -1.535111    0.027922
     22          1           0        4.631589    0.965076    0.095543
     23          1           0        2.563607    2.236180    0.074108
     24          6           0       -0.045588    2.724910   -0.067154
     25          1           0       -0.325143    3.147649    0.907963
     26          1           0        0.910521    3.164804   -0.351021
     27          1           0       -0.780583    3.080462   -0.796660
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3936007      0.4479586
0.3398302
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9546337100 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
```

This journal is © The Royal Society of Chemistry 2014

```
 Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860612620     A.U. after   13 cycles
            Convg  =    0.5282D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000118069	-0.000105969	-0.000017569
2	6	0.000139181	-0.000107230	0.000024342
3	6	0.000069804	-0.000105698	-0.000013890
4	6	-0.000054756	0.000081094	0.000154331
5	6	-0.000105178	0.000048199	0.000003375
6	6	-0.000124396	0.000006011	-0.000037304
7	6	0.000038062	-0.000063704	-0.000150599
8	6	-0.000040371	0.000146019	0.000122655
9	6	-0.000055530	0.000127971	-0.000231226
10	6	-0.000000427	-0.000088562	0.000000683
11	6	0.000009223	-0.000205128	0.000040547
12	1	-0.000032198	0.000096335	0.000002001
13	6	0.000172881	0.000071212	-0.000034297
14	6	0.000071916	0.000098819	-0.000016243
15	6	-0.000175217	0.000032231	0.000063573
16	1	-0.000043300	0.000080216	0.000154487
17	1	0.000060506	0.000076312	0.000039256
18	1	-0.000071417	0.000073316	0.000001715
19	1	0.000030020	-0.000183235	-0.000130990
20	1	0.000087293	0.000014128	-0.000064079
21	1	-0.000098868	-0.000019385	0.000049645
22	1	-0.000061157	-0.000066303	-0.000087914
23	1	0.000005268	-0.000047097	-0.000111405
24	6	0.000255098	-0.000171759	0.000175577
25	1	-0.000003213	-0.000018531	0.000084901
26	1	0.000214371	0.000222282	0.000086730
27	1	-0.000169526	0.000008456	-0.000108303

Cartesian Forces: Max 0.000255098 RMS 0.000103150

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal Forces: Max 0.000445696 RMS 0.000100809
Search for a local minimum.
Step number 36 out of a maximum of 157
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 13 14 15 16
17
18 19 21 20
23
22 25 24 27
26
28 29 30 31
32
33 35 36

This journal is © The Royal Society of Chemistry 2014

```
 Use linear search instead of GDIIS.
     Eigenvalues ---    0.00001   0.00385   0.01531   0.01621
0.01788
     Eigenvalues ---    0.01814   0.01835   0.01876   0.01905
0.01974
     Eigenvalues ---    0.01976   0.02018   0.02071   0.02108
0.02115
     Eigenvalues ---    0.02144   0.02177   0.02224   0.02243
0.02337
     Eigenvalues ---    0.02404   0.04018   0.05539   0.06612
0.10106
     Eigenvalues ---    0.12378   0.14248   0.15559   0.15897
0.15970
     Eigenvalues ---    0.16000   0.16001   0.16002   0.16014
0.16199
     Eigenvalues ---    0.16429   0.19647   0.21743   0.22019
0.22535
     Eigenvalues ---    0.22929   0.23288   0.24347   0.24645
0.25218
     Eigenvalues ---    0.26741   0.30346   0.31948   0.33010
0.33416
     Eigenvalues ---    0.33606   0.33631   0.33642   0.33682
0.33685
     Eigenvalues ---    0.33777   0.34154   0.34608   0.36529
0.37346
     Eigenvalues ---    0.37908   0.38187   0.38760   0.39736
0.40478
     Eigenvalues ---    0.41109   0.42269   0.43313   0.45056
0.47891
     Eigenvalues ---    0.48842   0.49857   0.51210   0.51805
0.91992
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-9.51115401D-05 EMin= 1.21587918D-05
 Quartic linear search produced a step of -0.00004.
 Maximum step size (   0.071) exceeded in Quadratic search.
    -- Step size scaled by   0.079
 Iteration  1 RMS(Cart)=  0.00844478 RMS(Int)=  0.00010785
 Iteration  2 RMS(Cart)=  0.00011205 RMS(Int)=  0.00000097
 Iteration  3 RMS(Cart)=  0.00000002 RMS(Int)=  0.00000097
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.59035   0.00004   0.00000  -0.00019  -0.00019
2.59015
    R2        2.69185   0.00001   0.00000   0.00013   0.00013
2.69199
    R3        2.05427  -0.00010   0.00000   0.00039   0.00039
2.05466
    R4        2.70434   0.00003   0.00000   0.00029   0.00029
2.70462
    R5        2.05621  -0.00010   0.00000  -0.00003  -0.00003
2.05618
    R6        2.73131   0.00020   0.00000  -0.00073  -0.00073
2.73059
    R7        2.64284   0.00000   0.00000   0.00030   0.00030
2.64314
    R8        2.71079   0.00012   0.00000  -0.00082  -0.00082
2.70997
    R9        2.67924   0.00025   0.00000  -0.00028  -0.00028
2.67895
   R10        2.59537   0.00002   0.00000   0.00059   0.00059
2.59596
   R11        2.04978  -0.00017   0.00000   0.00072   0.00072
2.05051
   R12        2.05467  -0.00009   0.00000  -0.00008  -0.00008
2.05459
   R13        2.64137  -0.00004   0.00000   0.00077   0.00077
2.64214
   R14        2.05728  -0.00009   0.00000  -0.00003  -0.00003
2.05725
   R15        2.67864  -0.00018   0.00000   0.00132   0.00132
2.67996
   R16        2.86254  -0.00013   0.00000  -0.00075  -0.00075
2.86180
```

This journal is © The Royal Society of Chemistry 2014

R17	2.73904	0.00004	0.00000	-0.00018	-0.00018
2.73886					
R18	2.71428	-0.00011	0.00000	-0.00019	-0.00019
2.71409					
R19	2.70590	0.00002	0.00000	0.00021	0.00021
2.70611					
R20	2.05618	-0.00010	0.00000	-0.00001	-0.00001
2.05617					
R21	2.58830	0.00012	0.00000	-0.00049	-0.00049
2.58780					
R22	2.69234	0.00006	0.00000	-0.00009	-0.00009
2.69224					
R23	2.05422	-0.00010	0.00000	0.00044	0.00044
2.05466					
R24	2.59366	0.00004	0.00000	0.00047	0.00047
2.59414					
R25	2.05464	-0.00009	0.00000	-0.00009	-0.00009
2.05456					
R26	2.04837	-0.00005	0.00000	0.00048	0.00048
2.04885					
R27	2.07673	0.00008	0.00000	-0.00077	-0.00077
2.07596					
R28	2.05991	0.00027	0.00000	-0.00068	-0.00068
2.05923					
R29	2.06907	0.00020	0.00000	-0.00028	-0.00028
2.06879					
A1	2.09047	-0.00001	0.00000	0.00063	0.00063
2.09109					
A2	2.10202	-0.00001	0.00000	0.00095	0.00095
2.10298					
A3	2.09069	0.00002	0.00000	-0.00158	-0.00158
2.08911					
A4	2.11545	0.00001	0.00000	-0.00090	-0.00090
2.11455					
A5	2.10444	-0.00003	0.00000	0.00186	0.00186
2.10630					
A6	2.06328	0.00002	0.00000	-0.00096	-0.00096
2.06232					
A7	2.08407	0.00004	0.00000	-0.00002	-0.00001
2.08405					
A8	2.11568	-0.00007	0.00000	0.00013	0.00012
2.11581					
A9	2.08343	0.00002	0.00000	-0.00011	-0.00011
2.08332					
A10	2.04725	-0.00012	0.00000	0.00135	0.00135
2.04860					
A11	2.09736	-0.00011	0.00000	0.00035	0.00035
2.09770					
A12	2.13854	0.00023	0.00000	-0.00173	-0.00173
2.13681					
A13	2.12254	0.00005	0.00000	-0.00130	-0.00130
2.12124					

This journal is © The Royal Society of Chemistry 2014

A14	2.08518	0.00005	0.00000	-0.00009	-0.00010
2.08508					
A15	2.07536	-0.00010	0.00000	0.00142	0.00142
2.07678					
A16	2.10643	0.00003	0.00000	0.00023	0.00023
2.10666					
A17	2.08596	0.00000	0.00000	-0.00098	-0.00098
2.08498					
A18	2.09079	-0.00002	0.00000	0.00075	0.00075
2.09154					
A19	2.11889	0.00001	0.00000	-0.00013	-0.00013
2.11875					
A20	2.08257	0.00000	0.00000	0.00002	0.00002
2.08259					
A21	2.08170	-0.00001	0.00000	0.00010	0.00010
2.08180					
A22	2.08781	-0.00001	0.00000	0.00038	0.00038
2.08818					
A23	2.07579	0.00045	0.00000	-0.00242	-0.00242
2.07338					
A24	2.11956	-0.00044	0.00000	0.00204	0.00204
2.12160					
A25	2.08879	0.00010	0.00000	-0.00088	-0.00088
2.08792					
A26	2.15402	-0.00018	0.00000	0.00012	0.00012
2.15414					
A27	2.04034	0.00008	0.00000	0.00077	0.00077
2.04111					
A28	2.08911	-0.00001	0.00000	0.00044	0.00044
2.08955					
A29	2.10823	0.00004	0.00000	-0.00062	-0.00062
2.10761					
A30	2.08584	-0.00003	0.00000	0.00018	0.00018
2.08602					
A31	2.06132	0.00003	0.00000	-0.00131	-0.00131
2.06001					
A32	2.11729	-0.00003	0.00000	-0.00069	-0.00069
2.11659					
A33	2.10456	0.00000	0.00000	0.00200	0.00200
2.10656					
A34	2.08834	0.00000	0.00000	0.00051	0.00051
2.08886					
A35	2.10328	-0.00002	0.00000	0.00109	0.00109
2.10438					
A36	2.09155	0.00002	0.00000	-0.00160	-0.00160
2.08995					
A37	2.10818	0.00000	0.00000	0.00045	0.00045
2.10863					
A38	2.08595	0.00002	0.00000	-0.00093	-0.00093
2.08502					
A39	2.08905	-0.00002	0.00000	0.00048	0.00048
2.08953					

This journal is © The Royal Society of Chemistry 2014

A40	2.12619	-0.00001	0.00000	-0.00115	-0.00116	2.12503
A41	2.08955	-0.00001	0.00000	-0.00006	-0.00007	2.08949
A42	2.06732	0.00003	0.00000	0.00127	0.00127	2.06859
A43	1.95035	-0.00011	0.00000	-0.00048	-0.00048	1.94988
A44	1.96538	-0.00004	0.00000	0.00043	0.00043	1.96581
A45	1.93861	0.00010	0.00000	-0.00095	-0.00095	1.93766
A46	1.87440	-0.00002	0.00000	-0.00193	-0.00193	1.87246
A47	1.87079	0.00000	0.00000	0.00055	0.00055	1.87134
A48	1.85901	0.00007	0.00000	0.00249	0.00249	1.86150
D1	-0.00109	0.00000	0.00000	-0.00049	-0.00049	-0.00158
D2	3.13471	0.00004	0.00000	-0.00114	-0.00114	3.13357
D3	-3.13863	-0.00002	0.00000	0.00041	0.00041	-3.13822
D4	-0.00283	0.00002	0.00000	-0.00023	-0.00023	-0.00306
D5	0.01080	-0.00006	0.00000	0.00003	0.00003	0.01083
D6	-3.12814	-0.00006	0.00000	0.00016	0.00016	-3.12798
D7	-3.13482	-0.00003	0.00000	-0.00086	-0.00086	-3.13568
D8	0.00943	-0.00004	0.00000	-0.00073	-0.00073	0.00870
D9	-0.01382	0.00007	0.00000	0.00005	0.00005	-0.01377
D10	3.12557	0.00007	0.00000	-0.00091	-0.00091	3.12466
D11	3.13343	0.00003	0.00000	0.00067	0.00067	3.13410
D12	-0.01036	0.00003	0.00000	-0.00029	-0.00029	-0.01065
D13	0.01872	-0.00008	0.00000	0.00084	0.00085	0.01957
D14	-3.13183	-0.00003	0.00000	-0.00248	-0.00248	-3.13431
D15	-3.12071	-0.00008	0.00000	0.00178	0.00178	-3.11892
D16	0.01193	-0.00003	0.00000	-0.00154	-0.00155	0.01038
D17	-3.12104	-0.00009	0.00000	0.00314	0.00314	-3.11790

This journal is © The Royal Society of Chemistry 2014

D18	0.01307	-0.00008	0.00000	0.00153	0.00153	0.01460
D19	0.01835	-0.00009	0.00000	0.00218	0.00218	0.02053
D20	-3.13073	-0.00008	0.00000	0.00058	0.00058	-3.13015
D21	-0.00951	0.00002	0.00000	-0.00132	-0.00132	-0.01083
D22	3.11621	0.00010	0.00000	0.00058	0.00058	3.11679
D23	3.14127	-0.00002	0.00000	0.00208	0.00208	-3.13984
D24	-0.01620	0.00006	0.00000	0.00398	0.00398	-0.01222
D25	-0.04349	0.00017	0.00000	0.00169	0.00169	-0.04180
D26	3.10536	0.00019	0.00000	0.00178	0.00178	3.10715
D27	3.08866	0.00022	0.00000	-0.00179	-0.00179	3.08687
D28	-0.04567	0.00024	0.00000	-0.00170	-0.00170	-0.04737
D29	-0.00521	0.00005	0.00000	0.00090	0.00090	-0.00431
D30	3.13372	0.00005	0.00000	0.00077	0.00077	3.13449
D31	-3.13101	-0.00004	0.00000	-0.00097	-0.00098	-3.13199
D32	0.00792	-0.00003	0.00000	-0.00111	-0.00111	0.00681
D33	-0.01655	0.00008	0.00000	-0.00292	-0.00292	-0.01947
D34	3.12219	0.00007	0.00000	-0.00207	-0.00207	3.12012
D35	3.13253	0.00006	0.00000	-0.00132	-0.00132	3.13121
D36	-0.01192	0.00005	0.00000	-0.00046	-0.00046	-0.01238
D37	0.04513	-0.00018	0.00000	-0.00244	-0.00244	0.04269
D38	-3.08855	-0.00017	0.00000	-0.00414	-0.00414	-3.09269
D39	-3.10391	-0.00020	0.00000	-0.00256	-0.00255	-3.10647
D40	0.04560	-0.00019	0.00000	-0.00426	-0.00426	0.04134
D41	1.30222	-0.00001	0.00000	-0.02700	-0.02700	1.27521
D42	-2.86944	-0.00014	0.00000	-0.02955	-0.02955	-2.89898
D43	-0.78604	-0.00001	0.00000	-0.02673	-0.02673	-0.81278

This journal is © The Royal Society of Chemistry 2014

D44	-1.83198	0.00001	0.00000	-0.02690	-0.02690	-1.85888
D45	0.27955	-0.00012	0.00000	-0.02945	-0.02945	0.25011
D46	2.36295	0.00001	0.00000	-0.02663	-0.02663	2.33631
D47	-0.01555	0.00006	0.00000	0.00305	0.00305	-0.01250
D48	3.12886	0.00007	0.00000	0.00220	0.00220	3.13107
D49	3.11864	0.00005	0.00000	0.00464	0.00464	3.12327
D50	-0.02014	0.00006	0.00000	0.00379	0.00379	-0.01635
D51	-3.13860	-0.00001	0.00000	-0.00081	-0.00081	-3.13941
D52	0.02032	-0.00009	0.00000	-0.00456	-0.00456	0.01577
D53	0.01071	0.00000	0.00000	-0.00246	-0.00246	0.00825
D54	-3.11356	-0.00007	0.00000	-0.00621	-0.00621	-3.11977
D55	0.01140	-0.00002	0.00000	-0.00332	-0.00332	0.00809
D56	-3.12415	-0.00005	0.00000	-0.00345	-0.00345	-3.12759
D57	-3.13304	-0.00003	0.00000	-0.00247	-0.00246	-3.13550
D58	0.01460	-0.00006	0.00000	-0.00259	-0.00259	0.01201
D59	0.00135	0.00001	0.00000	-0.00016	-0.00016	0.00119
D60	3.13874	0.00002	0.00000	0.00091	0.00091	3.13965
D61	-3.13406	-0.00003	0.00000	-0.00028	-0.00028	-3.13433
D62	0.00334	-0.00002	0.00000	0.00079	0.00079	0.00413
D63	-0.01133	0.00005	0.00000	0.00160	0.00160	-0.00973
D64	3.12689	0.00006	0.00000	0.00177	0.00177	3.12866
D65	3.13443	0.00004	0.00000	0.00053	0.00053	3.13496
D66	-0.01054	0.00005	0.00000	0.00070	0.00070	-0.00984
D67	0.00495	-0.00006	0.00000	-0.00021	-0.00021	0.00474
D68	3.12943	0.00002	0.00000	0.00348	0.00348	3.13291
D69	-3.13326	-0.00006	0.00000	-0.00038	-0.00038	-3.13364

```
   D70       -0.00878   0.00001   0.00000   0.00331   0.00331  -
0.00547
         Item               Value     Threshold  Converged?
 Maximum Force            0.000446     0.000450     YES
 RMS     Force            0.000101     0.000300     YES
 Maximum Displacement     0.061028     0.001800     NO
 RMS     Displacement     0.008445     0.001200     NO
 Predicted change in Energy=-7.483453D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792875   -5.419822    0.022598
      2          6           0       -3.422956   -5.393519   -0.013660
      3          6           0       -2.706326   -4.154735   -0.029738
      4          6           0       -3.440533   -2.910213   -0.024675
      5          6           0       -4.871674   -2.989071    0.021479
      6          6           0       -5.524270   -4.197619    0.046830
      7          6           0       -1.308032   -4.126097   -0.046486
      8          6           0       -2.747672   -1.673668   -0.049316
      9          6           0       -1.329705   -1.663579   -0.027464
     10          6           0       -0.604053   -2.918162   -0.033948
     11          6           0        0.827871   -2.905111   -0.024959
     12          1           0        1.348008   -3.860754   -0.035950
     13          6           0        1.527865   -1.728483    0.003729
     14          6           0        0.824702   -0.489640    0.026637
     15          6           0       -0.547611   -0.459508    0.008849
     16          1           0       -0.755687   -5.064104   -0.061148
     17          1           0       -5.326281   -6.367147    0.037667
     18          1           0       -2.849981   -6.318450   -0.025010
     19          1           0       -5.455961   -2.075180    0.050059
     20          1           0       -6.610366   -4.225131    0.088441
     21          1           0        2.615105   -1.731888    0.012093
     22          1           0        1.383904    0.442093    0.061629
     23          1           0       -1.044673    0.503672    0.035607
     24          6           0       -3.548910   -0.389203   -0.088900
     25          1           0       -4.025230   -0.177217    0.878054
     26          1           0       -2.940117    0.477014   -0.346738
     27          1           0       -4.345971   -0.446492   -0.837167
 ---------------------------------------------------------------------
                   Distance matrix (angstroms):
                    1          2          3          4          5
     1  C    0.000000
     2  C    1.370651   0.000000
     3  C    2.440671   1.431225   0.000000
     4  C    2.851176   2.483393   1.444964   0.000000
     5  C    2.432029   2.807381   2.459700   1.434055   0.000000
```

This journal is © The Royal Society of Chemistry 2014

6	C	1.424537	2.418544	2.819310	2.450405	1.373722
7	C	3.717880	2.465835	1.398688	2.454875	3.741255
8	C	4.268688	3.780816	2.481488	1.417641	2.499336
9	C	5.109346	4.277189	2.846216	2.451469	3.782178
10	C	4.879317	3.751536	2.438992	2.836506	4.268570
11	C	6.157826	4.925630	3.748617	4.268407	5.700352
12	H	6.335974	5.011184	4.064984	4.881986	6.280731
13	C	7.319707	6.159824	4.880184	5.107081	6.522538
14	C	7.474215	6.487855	5.089623	4.904492	6.220601
15	C	6.528949	5.710743	4.279748	3.791580	5.009628
16	H	4.053694	2.687954	2.152425	3.442234	4.610199
17	H	1.087278	2.138511	3.429792	3.938315	3.408567
18	H	2.141176	1.088084	2.168484	3.459022	3.895403
19	H	3.409849	3.892113	3.448392	2.182845	1.085083
20	H	2.175981	3.396341	3.906462	3.433606	2.134334
21	H	8.275213	7.061614	5.847185	6.169324	7.591604
22	H	8.515643	7.560816	6.153792	5.875423	7.134897
23	H	7.009778	6.358894	4.946324	4.171138	5.181254
24	C	5.183340	5.006466	3.859103	2.524155	2.919109
25	H	5.367121	5.326133	4.287685	2.937015	3.058873
26	H	6.192076	5.899766	4.648467	3.439105	3.985002
27	H	5.066847	5.099333	4.134180	2.747705	2.734657

		6	7	8	9	10
6	C	0.000000				
7	C	4.217877	0.000000			
8	C	3.753540	2.843762	0.000000		
9	C	4.901148	2.462687	1.418172	0.000000	
10	C	5.084493	1.398160	2.478730	1.449341	0.000000
11	C	6.482701	2.460356	3.781739	2.489285	1.432011
12	H	6.881027	2.669282	4.643073	3.463784	2.167724
13	C	7.472021	3.713946	4.276218	2.858477	2.441686
14	C	7.352480	4.216364	3.764246	2.454084	2.818285
15	C	6.224311	3.745020	2.513531	1.436237	2.459674
16	H	4.847869	1.088649	3.932328	3.448797	2.151465
17	H	2.178563	4.601707	5.355888	6.172553	5.848082
18	H	3.413928	2.680388	4.645972	4.896843	4.075075
19	H	2.123540	4.628271	2.739692	4.147459	4.925310
20	H	1.087241	5.304975	4.631344	5.870295	6.148085
21	H	8.504732	4.596376	5.363445	3.945600	3.431085
22	H	8.321659	5.303448	4.643132	3.435908	3.905434
23	H	6.493770	4.637980	2.765543	2.186824	3.450787
24	C	4.292377	4.357489	1.514397	2.559820	3.882117
25	H	4.370547	4.881761	2.175209	3.208597	4.477608
26	H	5.355832	4.893106	2.179662	2.697685	4.133068
27	H	4.029987	4.836708	2.163615	3.351833	4.555904

		11	12	13	14	15
11	C	0.000000				
12	H	1.088080	0.000000			
13	C	1.369405	2.140212	0.000000		
14	C	2.416025	3.412064	1.424674	0.000000	
15	C	2.806077	3.894080	2.432678	1.372759	0.000000
16	H	2.677726	2.423679	4.042919	4.840564	4.609826

This journal is © The Royal Society of Chemistry 2014

17	H	7.061388	7.129766	8.276333	8.507632	7.598468
18	H	5.017716	4.864515	6.343041	6.890646	6.295177
19	H	6.338844	7.034889	6.992580	6.477748	5.167591
20	H	7.555308	7.967683	8.513004	8.320935	7.137454
21	H	2.138231	2.477885	1.087277	2.179205	3.409067
22	H	3.394178	4.304103	2.176114	1.087224	2.132233
23	H	3.889716	4.977777	3.406095	2.116911	1.084206
24	C	5.048771	6.002856	5.251276	4.376291	3.003714
25	H	5.639985	6.578415	5.831616	4.934001	3.595698
26	H	5.073465	6.107442	4.994988	3.904829	2.593762
27	H	5.785597	6.687342	6.070631	5.242507	3.891459

		16	17	18	19	20
16	H	0.000000				
17	H	4.753737	0.000000			
18	H	2.441467	2.477571	0.000000		
19	H	5.571230	4.293943	4.980171	0.000000	
20	H	5.916377	2.497936	4.305270	2.440577	0.000000
21	H	4.740387	9.195210	7.134781	8.078453	9.556747
22	H	5.908564	9.559963	7.977357	7.288384	9.257000
23	H	5.576111	8.095698	7.057207	5.109809	7.303514
24	C	5.445876	6.237858	5.970640	2.549249	4.911039
25	H	5.954299	6.380769	6.317553	2.516908	4.867445
26	H	5.962993	7.258380	6.803673	3.605636	5.980826
27	H	5.900398	6.064693	6.113713	2.161452	4.501372

		21	22	23	24	25
21	H	0.000000				
22	H	2.498900	0.000000			
23	H	4.288620	2.429497	0.000000		
24	C	6.309365	5.004634	2.661566	0.000000	
25	H	6.874660	5.505346	3.171286	1.098553	0.000000
26	H	5.989032	4.343402	1.933806	1.089698	1.762273
27	H	7.129521	5.867613	3.544449	1.094757	1.765606

		26	27
26	H	0.000000	
27	H	1.752087	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.652754	-1.002235	0.023224
2	6	0	-2.454741	-1.667186	-0.012697
3	6	0	-1.212963	-0.955648	-0.022860
4	6	0	-1.223050	0.489240	-0.012081
5	6	0	-2.500419	1.139443	0.033480
6	6	0	-3.671662	0.421865	0.053067

This journal is © The Royal Society of Chemistry 2014

```
      7          6           0        0.010712   -1.632906   -0.039255
      8          6           0       -0.002930    1.210811   -0.030821
      9          6           0        1.228349    0.507480   -0.008701
     10          6           0        1.225989   -0.941807   -0.020948
     11          6           0        2.470857   -1.649533   -0.011676
     12          1           0        2.440876   -2.737091   -0.027062
     13          6           0        3.666930   -0.983572    0.022634
     14          6           0        3.680794    0.440747    0.051236
     15          6           0        2.509181    1.155921    0.033375
     16          1           0        0.017448   -2.721369   -0.058225
     17          1           0       -4.589734   -1.553713    0.033771
     18          1           0       -2.423607   -2.754713   -0.028290
     19          1           0       -2.546922    2.223034    0.066250
     20          1           0       -4.624843    0.943241    0.094380
     21          1           0        4.605451   -1.532459    0.031151
     22          1           0        4.632130    0.965590    0.090679
     23          1           0        2.562864    2.238348    0.064566
     24          6           0       -0.050820    2.724075   -0.064512
     25          1           0       -0.358712    3.142721    0.903350
     26          1           0        0.911237    3.168524   -0.318195
     27          1           0       -0.767027    3.077714   -0.813164
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3936818      0.4480296
0.3398711
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9864985895 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860612279     A.U. after   11 cycles
             Convg  =    0.3742D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000395986   -0.000277950    0.000041249
      2        6           0.000342075    0.000171916   -0.000038098
      3        6           0.000209482   -0.000337133   -0.000100474
      4        6           0.000199793    0.000373614    0.000536574
      5        6          -0.000502716   -0.000311529   -0.000207605
      6        6          -0.000049706    0.000235243   -0.000058976
      7        6          -0.000016876    0.000262926    0.000048013
```

```
      8        6           0.000487857    0.000044408    0.000157673
      9        6          -0.000854060    0.000157075   -0.000371501
     10        6          -0.000001339   -0.000420764   -0.000099664
     11        6          -0.000358403   -0.000352701    0.000004400
     12        1           0.000131626    0.000197300   -0.000047444
     13        6           0.000568777    0.000267344   -0.000006602
     14        6          -0.000198418    0.000240551    0.000003686
     15        6           0.000099749   -0.000058046   -0.000033356
     16        1          -0.000026263    0.000089115    0.000193528
     17        1           0.000231812    0.000124448    0.000024271
     18        1          -0.000219342   -0.000014016   -0.000022089
     19        1           0.000103631   -0.000492815   -0.000110665
     20        1           0.000053190    0.000089141   -0.000053741
     21        1          -0.000243597   -0.000151014    0.000077661
     22        1          -0.000102287    0.000000228   -0.000113800
     23        1           0.000241179   -0.000201911    0.000022492
     24        6           0.000639935   -0.000075331    0.000307201
     25        1          -0.000164038   -0.000066463    0.000248975
     26        1           0.000149919    0.000362129   -0.000119863
     27        1          -0.000325995    0.000144236   -0.000281844
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000854060 RMS     0.000256744


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000673557 RMS     0.000184843
 Search for a local minimum.
 Step number  37 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   13   18   19   21
20
                                                     23   22   25   24
27
                                                     26   28   29   30
31
                                                     32   33   35   34
36
                                                     37
 DE=  3.41D-07 DEPred=-7.48D-06 R=-4.55D-02
 Trust test=-4.55D-02 RLast= 7.07D-02 DXMaxT set to 5.00D-02
     Eigenvalues ---    0.00001   0.01129   0.01536   0.01673
0.01801
     Eigenvalues ---    0.01813   0.01837   0.01889   0.01970
0.01973
     Eigenvalues ---    0.02002   0.02023   0.02071   0.02103
0.02126
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02143   0.02186   0.02220   0.02257
0.02310
     Eigenvalues ---    0.02453   0.02548   0.05948   0.06747
0.11766
     Eigenvalues ---    0.12681   0.15460   0.15593   0.15861
0.15974
     Eigenvalues ---    0.16000   0.16000   0.16003   0.16015
0.16162
     Eigenvalues ---    0.16442   0.20849   0.21956   0.22067
0.22541
     Eigenvalues ---    0.22930   0.23196   0.24348   0.24637
0.25237
     Eigenvalues ---    0.27621   0.30003   0.31292   0.33246
0.33471
     Eigenvalues ---    0.33610   0.33631   0.33682   0.33684
0.33712
     Eigenvalues ---    0.33994   0.34340   0.34570   0.36813
0.37125
     Eigenvalues ---    0.37774   0.38205   0.38691   0.39663
0.40476
     Eigenvalues ---    0.40973   0.42069   0.43591   0.45054
0.47338
     Eigenvalues ---    0.49273   0.49831   0.51177   0.51828
0.57561
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   5.59D-06 Eigenvector:
                           D44       D46       D45       D41       D43
   1                     0.43318   0.41114   0.40860   0.40760
0.38556
                           D42       D39       D40       D26       A24
   1                     0.38302  -0.04185  -0.04139   0.03743  -
0.03512
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    37   36
 RFO step:  Lambda=-1.02621964D-05.
 DIIS coeffs:      0.47191      0.52809
 Iteration  1 RMS(Cart)=  0.00874684 RMS(Int)=  0.00001650
 Iteration  2 RMS(Cart)=  0.00002904 RMS(Int)=  0.00000181
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000181
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59015   0.00009   0.00010   0.00014   0.00024
2.59040
    R2        2.69199  -0.00004  -0.00007  -0.00024  -0.00031
2.69167
    R3        2.05466  -0.00022  -0.00020   0.00000  -0.00021
2.05445
    R4        2.70462  -0.00002  -0.00015   0.00000  -0.00016
2.70447
    R5        2.05618  -0.00010   0.00001  -0.00007  -0.00006
2.05612
    R6        2.73059   0.00032   0.00038   0.00037   0.00075
2.73134
    R7        2.64314  -0.00018  -0.00016  -0.00034  -0.00050
2.64264
    R8        2.70997   0.00048   0.00043  -0.00021   0.00022
2.71019
    R9        2.67895   0.00049   0.00015  -0.00034  -0.00019
2.67876
   R10        2.59596  -0.00025  -0.00031   0.00006  -0.00025
2.59571
   R11        2.05051  -0.00047  -0.00038  -0.00004  -0.00042
2.05009
   R12        2.05459  -0.00006   0.00004   0.00008   0.00013
2.05472
   R13        2.64214  -0.00038  -0.00040   0.00000  -0.00040
2.64173
   R14        2.05725  -0.00009   0.00002  -0.00004  -0.00002
2.05723
   R15        2.67996  -0.00059  -0.00070   0.00067  -0.00003
2.67993
   R16        2.86180   0.00015   0.00040  -0.00033   0.00006
2.86186
   R17        2.73886   0.00013   0.00009   0.00000   0.00010
2.73896
```

This journal is © The Royal Society of Chemistry 2014

R18	2.71409	0.00002	0.00010	-0.00019	-0.00009
2.71401					
R19	2.70611	0.00002	-0.00011	-0.00017	-0.00028
2.70583					
R20	2.05617	-0.00011	0.00000	-0.00007	-0.00006
2.05611					
R21	2.58780	0.00026	0.00026	0.00018	0.00045
2.58825					
R22	2.69224	0.00007	0.00005	-0.00044	-0.00039
2.69185					
R23	2.05466	-0.00024	-0.00023	0.00002	-0.00021
2.05444					
R24	2.59414	-0.00023	-0.00025	0.00018	-0.00007
2.59406					
R25	2.05456	-0.00006	0.00005	0.00009	0.00013
2.05469					
R26	2.04885	-0.00029	-0.00025	-0.00016	-0.00041
2.04844					
R27	2.07596	0.00028	0.00041	0.00006	0.00046
2.07643					
R28	2.05923	0.00040	0.00036	0.00053	0.00089
2.06012					
R29	2.06879	0.00042	0.00015	0.00021	0.00035
2.06915					
A1	2.09109	-0.00008	-0.00033	-0.00021	-0.00054
2.09055					
A2	2.10298	-0.00010	-0.00050	0.00072	0.00021
2.10319					
A3	2.08911	0.00019	0.00084	-0.00050	0.00033
2.08944					
A4	2.11455	0.00015	0.00048	0.00004	0.00051
2.11506					
A5	2.10630	-0.00027	-0.00098	0.00054	-0.00044
2.10585					
A6	2.06232	0.00012	0.00051	-0.00057	-0.00006
2.06226					
A7	2.08405	0.00005	0.00001	0.00020	0.00021
2.08426					
A8	2.11581	-0.00005	-0.00007	-0.00035	-0.00041
2.11539					
A9	2.08332	0.00000	0.00006	0.00015	0.00021
2.08353					
A10	2.04860	-0.00041	-0.00072	-0.00038	-0.00109
2.04751					
A11	2.09770	-0.00015	-0.00018	0.00002	-0.00017
2.09754					
A12	2.13681	0.00056	0.00091	0.00038	0.00129
2.13811					
A13	2.12124	0.00030	0.00069	0.00024	0.00092
2.12216					
A14	2.08508	0.00003	0.00005	0.00045	0.00051
2.08559					

This journal is © The Royal Society of Chemistry 2014

A15	2.07678	-0.00033	-0.00075	-0.00066	-0.00141
2.07538					
A16	2.10666	-0.00001	-0.00012	0.00018	0.00006
2.10672					
A17	2.08498	0.00009	0.00052	-0.00039	0.00013
2.08511					
A18	2.09154	-0.00009	-0.00040	0.00022	-0.00018
2.09136					
A19	2.11875	0.00006	0.00007	0.00013	0.00019
2.11895					
A20	2.08259	-0.00001	-0.00001	-0.00011	-0.00012
2.08247					
A21	2.08180	-0.00005	-0.00005	-0.00001	-0.00007
2.08174					
A22	2.08818	-0.00012	-0.00020	0.00005	-0.00016
2.08802					
A23	2.07338	0.00067	0.00128	0.00051	0.00179
2.07517					
A24	2.12160	-0.00055	-0.00108	-0.00055	-0.00162
2.11998					
A25	2.08792	0.00021	0.00046	0.00009	0.00055
2.08847					
A26	2.15414	-0.00008	-0.00006	0.00015	0.00010
2.15424					
A27	2.04111	-0.00014	-0.00041	-0.00024	-0.00065
2.04047					
A28	2.08955	0.00000	-0.00023	-0.00004	-0.00028
2.08927					
A29	2.10761	0.00005	0.00033	-0.00018	0.00015
2.10776					
A30	2.08602	-0.00005	-0.00009	0.00023	0.00013
2.08615					
A31	2.06001	0.00017	0.00069	-0.00050	0.00019
2.06020					
A32	2.11659	0.00008	0.00037	-0.00002	0.00034
2.11693					
A33	2.10656	-0.00026	-0.00106	0.00053	-0.00053
2.10604					
A34	2.08886	-0.00011	-0.00027	-0.00012	-0.00040
2.08846					
A35	2.10438	-0.00010	-0.00058	0.00067	0.00010
2.10447					
A36	2.08995	0.00021	0.00085	-0.00055	0.00030
2.09025					
A37	2.10863	-0.00006	-0.00024	0.00013	-0.00011
2.10852					
A38	2.08502	0.00012	0.00049	-0.00041	0.00008
2.08510					
A39	2.08953	-0.00006	-0.00025	0.00029	0.00003
2.08956					
A40	2.12503	0.00027	0.00061	0.00010	0.00071
2.12574					

A41	2.08949	-0.00001	0.00003	0.00028	0.00031	2.08980
A42	2.06859	-0.00026	-0.00067	-0.00034	-0.00101	2.06758
A43	1.94988	-0.00019	0.00025	-0.00168	-0.00143	1.94845
A44	1.96581	0.00012	-0.00023	0.00093	0.00070	1.96651
A45	1.93766	0.00022	0.00050	0.00222	0.00273	1.94039
A46	1.87246	0.00004	0.00102	-0.00118	-0.00016	1.87230
A47	1.87134	-0.00006	-0.00029	-0.00010	-0.00039	1.87095
A48	1.86150	-0.00015	-0.00132	-0.00027	-0.00159	1.85992
D1	-0.00158	0.00003	0.00026	0.00030	0.00056	-0.00102
D2	3.13357	0.00008	0.00060	0.00134	0.00194	3.13552
D3	-3.13822	-0.00003	-0.00022	-0.00024	-0.00046	-3.13868
D4	-0.00306	0.00003	0.00012	0.00080	0.00092	-0.00214
D5	0.01083	-0.00007	-0.00002	-0.00213	-0.00214	0.00868
D6	-3.12798	-0.00008	-0.00008	-0.00324	-0.00333	-3.13131
D7	-3.13568	-0.00002	0.00045	-0.00159	-0.00113	-3.13681
D8	0.00870	-0.00003	0.00039	-0.00270	-0.00232	0.00638
D9	-0.01377	0.00007	-0.00003	0.00260	0.00257	-0.01120
D10	3.12466	0.00008	0.00048	0.00320	0.00368	3.12834
D11	3.13410	0.00002	-0.00035	0.00158	0.00123	3.13533
D12	-0.01065	0.00003	0.00015	0.00218	0.00233	-0.00832
D13	0.01957	-0.00012	-0.00045	-0.00363	-0.00407	0.01549
D14	-3.13431	0.00002	0.00131	-0.00167	-0.00036	-3.13467
D15	-3.11892	-0.00013	-0.00094	-0.00421	-0.00515	-3.12408
D16	0.01038	0.00001	0.00082	-0.00226	-0.00144	0.00894
D17	-3.11790	-0.00018	-0.00166	-0.00449	-0.00615	-3.12405
D18	0.01460	-0.00011	-0.00081	-0.00404	-0.00485	0.00975

This journal is © The Royal Society of Chemistry 2014

D19	0.02053	-0.00017	-0.00115	-0.00390	-0.00505	0.01548
D20	-3.13015	-0.00010	-0.00030	-0.00344	-0.00375	-3.13390
D21	-0.01083	0.00008	0.00069	0.00189	0.00259	-0.00824
D22	3.11679	0.00013	-0.00031	0.00458	0.00428	3.12107
D23	-3.13984	-0.00006	-0.00110	-0.00010	-0.00120	-3.14104
D24	-0.01222	-0.00001	-0.00210	0.00258	0.00048	-0.01174
D25	-0.04180	0.00017	-0.00089	0.00894	0.00805	-0.03375
D26	3.10715	0.00017	-0.00094	0.00875	0.00780	3.11495
D27	3.08687	0.00032	0.00095	0.01099	0.01194	3.09881
D28	-0.04737	0.00031	0.00090	0.01080	0.01170	-0.03568
D29	-0.00431	0.00002	-0.00048	0.00097	0.00050	-0.00381
D30	3.13449	0.00002	-0.00041	0.00209	0.00169	3.13618
D31	-3.13199	-0.00004	0.00052	-0.00171	-0.00120	-3.13318
D32	0.00681	-0.00003	0.00059	-0.00059	-0.00001	0.00680
D33	-0.01947	0.00014	0.00154	0.00328	0.00482	-0.01465
D34	3.12012	0.00012	0.00109	0.00411	0.00521	3.12533
D35	3.13121	0.00007	0.00070	0.00282	0.00352	3.13473
D36	-0.01238	0.00005	0.00024	0.00366	0.00390	-0.00848
D37	0.04269	-0.00019	0.00129	-0.00952	-0.00823	0.03446
D38	-3.09269	-0.00015	0.00219	-0.01103	-0.00884	-3.10153
D39	-3.10647	-0.00018	0.00135	-0.00932	-0.00797	-3.11444
D40	0.04134	-0.00013	0.00225	-0.01083	-0.00858	0.03276
D41	1.27521	-0.00005	0.01426	-0.01209	0.00217	1.27739
D42	-2.89898	-0.00004	0.01560	-0.01418	0.00143	-2.89756
D43	-0.81278	0.00000	0.01412	-0.01234	0.00178	-0.81100
D44	-1.85888	-0.00006	0.01421	-0.01229	0.00192	-1.85696

```
   D45        0.25011  -0.00005   0.01555  -0.01438   0.00117
0.25128
   D46        2.33631  -0.00001   0.01407  -0.01254   0.00152
2.33784
   D47       -0.01250   0.00003  -0.00161   0.00351   0.00190  -
0.01060
   D48        3.13107   0.00006  -0.00116   0.00268   0.00152
3.13259
   D49        3.12327  -0.00001  -0.00245   0.00492   0.00247
3.12575
   D50       -0.01635   0.00002  -0.00200   0.00410   0.00210  -
0.01425
   D51       -3.13941  -0.00002   0.00043  -0.00079  -0.00036  -
3.13977
   D52        0.01577  -0.00003   0.00241  -0.00361  -0.00121
0.01456
   D53        0.00825   0.00002   0.00130  -0.00226  -0.00096
0.00729
   D54       -3.11977   0.00001   0.00328  -0.00509  -0.00181  -
3.12157
   D55        0.00809   0.00002   0.00175  -0.00273  -0.00098
0.00711
   D56       -3.12759   0.00000   0.00182  -0.00372  -0.00191  -
3.12950
   D57       -3.13550   0.00000   0.00130  -0.00190  -0.00060  -
3.13610
   D58        0.01201  -0.00002   0.00137  -0.00289  -0.00152
0.01048
   D59        0.00119  -0.00001   0.00008  -0.00035  -0.00027
0.00092
   D60        3.13965  -0.00001  -0.00048   0.00021  -0.00028
3.13938
   D61       -3.13433  -0.00003   0.00015  -0.00136  -0.00122  -
3.13555
   D62        0.00413  -0.00004  -0.00042  -0.00081  -0.00123
0.00291
   D63       -0.00973   0.00004  -0.00084   0.00230   0.00146  -
0.00828
   D64        3.12866   0.00005  -0.00093   0.00352   0.00259
3.13124
   D65        3.13496   0.00005  -0.00028   0.00175   0.00147
3.13643
   D66       -0.00984   0.00005  -0.00037   0.00297   0.00260  -
0.00724
   D67        0.00474  -0.00005   0.00011  -0.00092  -0.00081
0.00393
   D68        3.13291  -0.00004  -0.00184   0.00187   0.00004
3.13295
   D69       -3.13364  -0.00006   0.00020  -0.00214  -0.00194  -
3.13558
   D70       -0.00547  -0.00004  -0.00175   0.00065  -0.00110  -
0.00657
```

```
         Item               Value     Threshold  Converged?
 Maximum Force            0.000674     0.000450     NO
 RMS     Force            0.000185     0.000300     YES
 Maximum Displacement     0.039210     0.001800     NO
 RMS     Displacement     0.008748     0.001200     NO
 Predicted change in Energy=-1.618623D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792859   -5.421249    0.018128
      2          6           0       -3.422649   -5.393663   -0.010131
      3          6           0       -2.706537   -4.154646   -0.023836
      4          6           0       -3.441233   -2.909943   -0.021687
      5          6           0       -4.872677   -2.990752    0.014109
      6          6           0       -5.524829   -4.199466    0.035559
      7          6           0       -1.308467   -4.126005   -0.036813
      8          6           0       -2.748397   -1.673450   -0.043605
      9          6           0       -1.330381   -1.663779   -0.026055
     10          6           0       -0.604472   -2.918285   -0.029296
     11          6           0        0.827317   -2.905123   -0.022764
     12          1           0        1.347657   -3.860650   -0.030655
     13          6           0        1.527818   -1.728368   -0.001219
     14          6           0        0.824663   -0.489669    0.016237
     15          6           0       -0.547660   -0.459949    0.001983
     16          1           0       -0.756154   -5.064093   -0.045723
     17          1           0       -5.325589   -6.368861    0.031034
     18          1           0       -2.849179   -6.318288   -0.018037
     19          1           0       -5.458795   -2.078119    0.036224
     20          1           0       -6.611307   -4.227256    0.067692
     21          1           0        2.614955   -1.731952    0.005601
     22          1           0        1.383813    0.442447    0.043118
     23          1           0       -1.043801    0.503573    0.024354
     24          6           0       -3.547363   -0.387332   -0.076037
     25          1           0       -4.018250   -0.178292    0.894491
     26          1           0       -2.938316    0.479344   -0.333728
     27          1           0       -4.348738   -0.438188   -0.820425
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1          2          3          4          5
    1  C    0.000000
    2  C    1.370779   0.000000
    3  C    2.441063   1.431143   0.000000
    4  C    2.852216   2.483817   1.445361   0.000000
    5  C    2.431811   2.806627   2.459320   1.434170   0.000000
    6  C    1.424373   2.418130   2.819274   2.451024   1.373591
    7  C    3.717750   2.465246   1.398424   2.455143   3.740987
```

This journal is © The Royal Society of Chemistry 2014

8	C	4.269618	3.780968	2.481628	1.417539	2.500236
9	C	5.109725	4.276666	2.845738	2.451252	3.782899
10	C	4.879515	3.750998	2.438708	2.836783	4.269041
11	C	6.157836	4.924957	3.748257	4.268553	5.700756
12	H	6.335912	5.010626	4.064845	4.882355	6.281025
13	C	7.320431	6.159675	4.880276	5.107642	6.523816
14	C	7.475095	6.487644	5.089503	4.904797	6.222146
15	C	6.529661	5.710276	4.279276	3.791542	5.011075
16	H	4.052977	2.687021	2.152107	3.442468	4.609564
17	H	1.087169	2.138664	3.430043	3.939250	3.408378
18	H	2.140999	1.088054	2.168347	3.459387	3.894621
19	H	3.408859	3.891127	3.448260	2.183080	1.084860
20	H	2.175967	3.396190	3.906518	3.434046	2.134162
21	H	8.275674	7.061235	5.847101	6.169750	7.592712
22	H	8.516739	7.560761	6.153756	5.875695	7.136621
23	H	7.011348	6.359049	4.946314	4.171557	5.183695
24	C	5.186565	5.008318	3.860359	2.525428	2.922735
25	H	5.371837	5.326648	4.286642	2.938409	3.068394
26	H	6.195171	5.901823	4.650120	3.440576	3.988021
27	H	5.072605	5.105973	4.140464	2.751567	2.736155

		6	7	8	9	10
6	C	0.000000				
7	C	4.217623	0.000000			
8	C	3.754410	2.844023	0.000000		
9	C	4.901724	2.462347	1.418157	0.000000	
10	C	5.084835	1.397946	2.479160	1.449393	0.000000
11	C	6.482938	2.460147	3.781955	2.489299	1.431865
12	H	6.881151	2.669352	4.643454	3.463835	2.167686
13	C	7.473119	3.714086	4.276778	2.859037	2.441997
14	C	7.353844	4.216159	3.764529	2.454494	2.818275
15	C	6.225538	3.744369	2.513544	1.436191	2.459191
16	H	4.847107	1.088640	3.932619	3.448515	2.151225
17	H	2.178529	4.601335	5.356713	6.172742	5.847997
18	H	3.413412	2.679600	4.646001	4.896046	4.074170
19	H	2.122375	4.628649	2.741603	4.149621	4.926928
20	H	1.087309	5.304837	4.632104	5.870978	6.148567
21	H	8.505622	4.596360	5.363897	3.946052	3.431226
22	H	8.323266	5.303349	4.643243	3.436252	3.905514
23	H	6.496023	4.637541	2.765808	2.186798	3.450362
24	C	4.295951	4.357966	1.514430	2.558676	3.881818
25	H	4.379199	4.877980	2.174407	3.206043	4.473792
26	H	5.358889	4.894263	2.180542	2.696867	4.133206
27	H	4.032755	4.843273	2.165736	3.353144	4.560295

		11	12	13	14	15
11	C	0.000000				
12	H	1.088047	0.000000			
13	C	1.369641	2.140082	0.000000		
14	C	2.415771	3.411633	1.424468	0.000000	
15	C	2.805362	3.893336	2.432388	1.372719	0.000000
16	H	2.677509	2.423741	4.042965	4.840266	4.609109
17	H	7.061064	7.129315	8.276739	8.508274	7.598993
18	H	5.016607	4.863494	6.342377	6.889927	6.294246

This journal is © The Royal Society of Chemistry 2014

19	H	6.340553	7.036311	6.995462	6.481159	5.170966
20	H	7.555750	7.968010	8.514373	8.322611	7.138959
21	H	2.138407	2.477643	1.087164	2.179111	3.408833
22	H	3.394150	4.303882	2.176039	1.087295	2.132276
23	H	3.888768	4.976800	3.405208	2.116071	1.083988
24	C	5.047765	6.002267	5.249899	4.374197	3.001595
25	H	5.635289	6.573325	5.827855	4.931743	3.594564
26	H	5.072604	6.107124	4.993086	3.901471	2.590407
27	H	5.789091	6.692227	6.072032	5.240871	3.889090

		16	17	18	19	20
16	H	0.000000				
17	H	4.752689	0.000000			
18	H	2.440190	2.477413	0.000000		
19	H	5.571138	4.292812	4.979164	0.000000	
20	H	5.915740	2.498177	4.305041	2.438865	0.000000
21	H	4.740271	9.195315	7.133849	8.081225	9.557945
22	H	5.908412	9.560865	7.976810	7.292090	9.258978
23	H	5.575532	8.097166	7.056839	5.114435	7.306144
24	C	5.446453	6.241173	5.972191	2.554395	4.914614
25	H	5.949480	6.385752	6.316564	2.533995	4.878693
26	H	5.964434	7.261545	6.805543	3.609750	5.983652
27	H	5.908115	6.070594	6.121118	2.157649	4.501668

		21	22	23	24	25
21	H	0.000000				
22	H	2.499026	0.000000			
23	H	4.287706	2.428456	0.000000		
24	C	6.307838	5.001922	2.659250	0.000000	
25	H	6.870472	5.503856	3.173235	1.098797	0.000000
26	H	5.986969	4.338683	1.928210	1.090170	1.762743
27	H	7.130860	5.863733	3.538809	1.094944	1.765702

		26	27
26	H	0.000000	
27	H	1.751579	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.653553	-1.002180	0.018164
2	6	0	-2.454889	-1.666597	-0.009907
3	6	0	-1.213206	-0.955023	-0.017449
4	6	0	-1.223130	0.490280	-0.009164
5	6	0	-2.501498	1.139411	0.026177
6	6	0	-3.672673	0.421872	0.041617
7	6	0	0.010039	-1.632590	-0.030231
8	6	0	-0.002821	1.211399	-0.024933

```
      9          6           0        1.228062    0.507280   -0.007282
     10          6           0        1.225467   -0.942080   -0.016707
     11          6           0        2.470041   -1.650054   -0.010056
     12          1           0        2.439918   -2.737611   -0.022659
     13          6           0        3.666856   -0.984621    0.017342
     14          6           0        3.681149    0.439580    0.040905
     15          6           0        2.509554    1.154788    0.026747
     16          1           0        0.016325   -2.721128   -0.043766
     17          1           0       -4.590275   -1.553923    0.026357
     18          1           0       -2.423548   -2.754128   -0.022370
     19          1           0       -2.549835    2.222867    0.052789
     20          1           0       -4.626125    0.943550    0.073571
     21          1           0        4.605018   -1.533923    0.024185
     22          1           0        4.632829    0.964482    0.072422
     23          1           0        2.564580    2.237039    0.053869
     24          6           0       -0.047421    2.724948   -0.051026
     25          1           0       -0.351995    3.138124    0.920507
     26          1           0        0.915242    3.169414   -0.304399
     27          1           0       -0.763993    3.086758   -0.795688
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3937845      0.4479680
0.3397987
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9612344546 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860634578     A.U. after   11 cycles
             Convg  =    0.4906D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000155052   -0.000207020    0.000038574
      2        6           0.000173397    0.000036373    0.000012458
      3        6          -0.000001091   -0.000149651   -0.000075417
      4        6           0.000088352    0.000042321    0.000296541
      5        6          -0.000445486   -0.000090659   -0.000019237
      6        6          -0.000126261    0.000154653   -0.000072210
      7        6           0.000093367    0.000106538    0.000052582
      8        6           0.000547943    0.000212800   -0.000103486
      9        6          -0.000597965    0.000137449   -0.000246259
```

```
     10        6           -0.000049447   -0.000230334   -0.000086883
     11        6           -0.000112611   -0.000224888    0.000039203
     12        1            0.000109206    0.000152986   -0.000030424
     13        6            0.000378782    0.000028999    0.000012905
     14        6           -0.000141529    0.000266892   -0.000046102
     15        6            0.000112347    0.000019548    0.000081475
     16        1           -0.000020809    0.000076825    0.000097663
     17        1            0.000208200    0.000062986    0.000005543
     18        1           -0.000179444   -0.000021542   -0.000012064
     19        1            0.000116890   -0.000258531   -0.000054886
     20        1            0.000100733    0.000095331   -0.000024523
     21        1           -0.000173480   -0.000159759    0.000035523
     22        1           -0.000141538   -0.000036188   -0.000060943
     23        1            0.000167766   -0.000113577    0.000017604
     24        6            0.000405506    0.000174890    0.000214812
     25        1           -0.000127040   -0.000077425    0.000103869
     26        1           -0.000001897    0.000047966    0.000025719
     27        1           -0.000228837   -0.000046982   -0.000202038
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000597965 RMS     0.000172511


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000380277 RMS     0.000101103
 Search for a local minimum.
 Step number  38 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   13   18   19   21
20
                                                     23   22   25   24
27
                                                     26   28   29   30
31
                                                     32   33   35   34
36
                                                     37   38
 DE= -2.23D-05 DEPred=-1.62D-05 R= 1.38D+00
 SS=  1.41D+00  RLast= 3.32D-02 DXNew= 8.4090D-02 9.9664D-02
 Trust test= 1.38D+00 RLast= 3.32D-02 DXMaxT set to 8.41D-02
     Eigenvalues ---    0.00000   0.00273   0.01046   0.01533
0.01670
     Eigenvalues ---    0.01796   0.01816   0.01831   0.01860
0.01930
     Eigenvalues ---    0.01975   0.01979   0.02040   0.02065
0.02102
     Eigenvalues ---    0.02118   0.02146   0.02172   0.02226
0.02230
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02344   0.02357   0.05495   0.06487
0.08620
     Eigenvalues ---    0.10098   0.15320   0.15715   0.15822
0.15902
     Eigenvalues ---    0.16000   0.16001   0.16004   0.16010
0.16065
     Eigenvalues ---    0.16450   0.18637   0.21066   0.22008
0.22539
     Eigenvalues ---    0.22652   0.23109   0.24298   0.24589
0.25139
     Eigenvalues ---    0.25574   0.29319   0.32526   0.32936
0.33241
     Eigenvalues ---    0.33592   0.33631   0.33678   0.33683
0.33683
     Eigenvalues ---    0.33919   0.34418   0.35481   0.36820
0.37203
     Eigenvalues ---    0.37871   0.38015   0.39522   0.39686
0.40546
     Eigenvalues ---    0.40699   0.41639   0.44288   0.45443
0.46111
     Eigenvalues ---    0.49760   0.49797   0.50332   0.51395
0.62129
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   1.99D-06 Eigenvector:
```

This journal is © The Royal Society of Chemistry 2014

```
                         D44       D45       D46       D41       D42
   1                   0.42034   0.41669   0.40564   0.40031
0.39666
                         D43       D38       D27       D37       D25
   1                   0.38562   0.04873  -0.04853   0.03779  -
0.03698
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    38   37   36
 RFO step:  Lambda=-5.34088158D-06.
 DIIS coeffs:      2.06303      0.07131     -1.13435
 Maximum step size (   0.084) exceeded in Quadratic search.
    -- Step size scaled by   0.077
 Iteration  1 RMS(Cart)=  0.00982588 RMS(Int)=  0.00014897
 Iteration  2 RMS(Cart)=  0.00015446 RMS(Int)=  0.00000067
 Iteration  3 RMS(Cart)=  0.00000003 RMS(Int)=  0.00000067
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59040  -0.00002   0.00000   0.00030   0.00031
2.59070
    R2        2.69167   0.00010  -0.00001  -0.00032  -0.00033
2.69134
    R3        2.05445  -0.00016   0.00002   0.00004   0.00006
2.05451
    R4        2.70447   0.00002   0.00001  -0.00022  -0.00021
2.70426
    R5        2.05612  -0.00008  -0.00001   0.00007   0.00007
2.05619
    R6        2.73134   0.00012   0.00000  -0.00020  -0.00020
2.73114
    R7        2.64264  -0.00002  -0.00001  -0.00025  -0.00026
2.64237
    R8        2.71019   0.00032  -0.00005  -0.00035  -0.00040
2.70979
    R9        2.67876   0.00038  -0.00004  -0.00040  -0.00044
2.67832
   R10        2.59571  -0.00014   0.00003   0.00001   0.00004
2.59575
   R11        2.05009  -0.00028   0.00003   0.00006   0.00009
2.05018
   R12        2.05472  -0.00010   0.00000   0.00022   0.00022
2.05493
   R13        2.64173  -0.00017   0.00003  -0.00023  -0.00020
2.64154
   R14        2.05723  -0.00008   0.00000   0.00010   0.00010
2.05733
   R15        2.67993  -0.00036   0.00011   0.00004   0.00015
2.68008
   R16        2.86186   0.00006  -0.00006   0.00038   0.00032
2.86218
   R17        2.73896   0.00018  -0.00001   0.00042   0.00041
2.73937
```

This journal is © The Royal Society of Chemistry 2014

R18	2.71401	0.00007	-0.00002	0.00003	0.00000
2.71401					
R19	2.70583	0.00007	0.00000	-0.00014	-0.00015
2.70568					
R20	2.05611	-0.00008	-0.00001	0.00007	0.00007
2.05618					
R21	2.58825	0.00005	-0.00001	0.00013	0.00013
2.58837					
R22	2.69185	0.00019	-0.00004	-0.00038	-0.00042
2.69143					
R23	2.05444	-0.00017	0.00002	0.00004	0.00006
2.05451					
R24	2.59406	-0.00016	0.00004	-0.00010	-0.00006
2.59400					
R25	2.05469	-0.00010	0.00000	0.00022	0.00022
2.05491					
R26	2.04844	-0.00018	0.00001	-0.00018	-0.00017
2.04827					
R27	2.07643	0.00013	-0.00003	0.00002	-0.00001
2.07641					
R28	2.06012	0.00003	0.00001	-0.00018	-0.00017
2.05995					
R29	2.06915	0.00031	0.00000	0.00057	0.00058
2.06972					
A1	2.09055	-0.00001	0.00001	0.00000	0.00001
2.09056					
A2	2.10319	-0.00015	0.00010	0.00018	0.00028
2.10347					
A3	2.08944	0.00016	-0.00011	-0.00018	-0.00029
2.08914					
A4	2.11506	0.00006	-0.00004	0.00010	0.00007
2.11513					
A5	2.10585	-0.00020	0.00013	-0.00010	0.00003
2.10588					
A6	2.06226	0.00014	-0.00009	0.00000	-0.00009
2.06217					
A7	2.08426	0.00003	0.00002	-0.00023	-0.00022
2.08404					
A8	2.11539	0.00002	-0.00002	0.00053	0.00051
2.11590					
A9	2.08353	-0.00005	0.00001	-0.00029	-0.00029
2.08324					
A10	2.04751	-0.00017	0.00003	0.00021	0.00024
2.04775					
A11	2.09754	-0.00003	0.00002	0.00052	0.00053
2.09807					
A12	2.13811	0.00020	-0.00005	-0.00071	-0.00076
2.13735					
A13	2.12216	0.00011	-0.00004	0.00010	0.00006
2.12222					
A14	2.08559	-0.00001	0.00003	-0.00023	-0.00020
2.08539					

This journal is © The Royal Society of Chemistry 2014

A15	2.07538	-0.00010	0.00001	0.00013	0.00013
2.07551					
A16	2.10672	-0.00002	0.00002	-0.00017	-0.00015
2.10657					
A17	2.08511	0.00011	-0.00008	-0.00010	-0.00018
2.08493					
A18	2.09136	-0.00008	0.00005	0.00028	0.00033
2.09169					
A19	2.11895	0.00004	0.00000	0.00007	0.00007
2.11902					
A20	2.08247	0.00000	-0.00001	-0.00001	-0.00002
2.08246					
A21	2.08174	-0.00004	0.00000	-0.00005	-0.00005
2.08169					
A22	2.08802	-0.00004	0.00002	-0.00005	-0.00004
2.08798					
A23	2.07517	0.00003	-0.00006	-0.00208	-0.00214
2.07303					
A24	2.11998	0.00000	0.00005	0.00214	0.00219
2.12217					
A25	2.08847	0.00004	-0.00003	-0.00037	-0.00040
2.08807					
A26	2.15424	0.00007	0.00002	0.00089	0.00091
2.15515					
A27	2.04047	-0.00011	0.00001	-0.00052	-0.00050
2.03996					
A28	2.08927	0.00005	0.00002	0.00022	0.00024
2.08951					
A29	2.10776	-0.00004	-0.00004	-0.00024	-0.00028
2.10749					
A30	2.08615	-0.00001	0.00003	0.00001	0.00004
2.08619					
A31	2.06020	0.00015	-0.00010	-0.00014	-0.00024
2.05996					
A32	2.11693	0.00004	-0.00003	0.00026	0.00023
2.11717					
A33	2.10604	-0.00019	0.00013	-0.00012	0.00001
2.10605					
A34	2.08846	-0.00005	0.00001	-0.00020	-0.00019
2.08827					
A35	2.10447	-0.00014	0.00010	0.00029	0.00040
2.10487					
A36	2.09025	0.00019	-0.00012	-0.00009	-0.00021
2.09004					
A37	2.10852	-0.00001	0.00003	-0.00002	0.00001
2.10853					
A38	2.08510	0.00011	-0.00007	-0.00015	-0.00023
2.08487					
A39	2.08956	-0.00010	0.00004	0.00018	0.00022
2.08978					
A40	2.12574	0.00014	-0.00004	0.00047	0.00043
2.12617					

This journal is © The Royal Society of Chemistry 2014

A41	2.08980	0.00003	0.00002	0.00030	0.00032
2.09012					
A42	2.06758	-0.00017	0.00003	-0.00077	-0.00074
2.06683					
A43	1.94845	-0.00010	-0.00016	-0.00060	-0.00076
1.94769					
A44	1.96651	0.00010	0.00010	0.00188	0.00198
1.96849					
A45	1.94039	-0.00005	0.00014	-0.00054	-0.00040
1.93998					
A46	1.87230	0.00004	-0.00018	0.00007	-0.00011
1.87219					
A47	1.87095	-0.00001	0.00002	-0.00041	-0.00039
1.87056					
A48	1.85992	0.00002	0.00009	-0.00048	-0.00039
1.85952					
D1	-0.00102	0.00001	0.00000	0.00037	0.00037	-
0.00065					
D2	3.13552	0.00004	0.00006	0.00074	0.00080
3.13631					
D3	-3.13868	-0.00002	0.00000	0.00017	0.00016	-
3.13851					
D4	-0.00214	0.00001	0.00006	0.00053	0.00059	-
0.00155					
D5	0.00868	-0.00004	-0.00017	-0.00023	-0.00040
0.00828					
D6	-3.13131	-0.00003	-0.00026	-0.00086	-0.00112	-
3.13243					
D7	-3.13681	-0.00002	-0.00017	-0.00003	-0.00020	-
3.13701					
D8	0.00638	-0.00001	-0.00025	-0.00066	-0.00092
0.00546					
D9	-0.01120	0.00004	0.00022	0.00036	0.00058	-
0.01062					
D10	3.12834	0.00003	0.00022	0.00113	0.00135
3.12969					
D11	3.13533	0.00001	0.00016	0.00001	0.00016
3.13550					
D12	-0.00832	0.00000	0.00017	0.00077	0.00094	-
0.00738					
D13	0.01549	-0.00005	-0.00026	-0.00119	-0.00145
0.01405					
D14	-3.13467	0.00000	-0.00025	0.00014	-0.00011	-
3.13478					
D15	-3.12408	-0.00004	-0.00027	-0.00194	-0.00221	-
3.12628					
D16	0.00894	0.00001	-0.00025	-0.00062	-0.00087
0.00807					
D17	-3.12405	-0.00007	-0.00023	-0.00213	-0.00236	-
3.12641					
D18	0.00975	-0.00005	-0.00026	-0.00107	-0.00134
0.00841					

This journal is © The Royal Society of Chemistry 2014

D19	0.01548	-0.00008	-0.00022	-0.00136	-0.00159	0.01390
D20	-3.13390	-0.00006	-0.00026	-0.00031	-0.00056	-3.13446
D21	-0.00824	0.00002	0.00010	0.00135	0.00144	-0.00679
D22	3.12107	0.00006	0.00040	0.00133	0.00173	3.12279
D23	-3.14104	-0.00004	0.00008	-0.00002	0.00007	-3.14097
D24	-0.01174	0.00000	0.00039	-0.00004	0.00035	-0.01139
D25	-0.03375	0.00007	0.00081	0.00256	0.00336	-0.03039
D26	3.11495	0.00010	0.00079	0.00052	0.00132	3.11627
D27	3.09881	0.00012	0.00082	0.00396	0.00478	3.10358
D28	-0.03568	0.00015	0.00081	0.00192	0.00273	-0.03294
D29	-0.00381	0.00003	0.00012	-0.00066	-0.00054	-0.00435
D30	3.13618	0.00002	0.00021	-0.00002	0.00018	3.13636
D31	-3.13318	-0.00001	-0.00018	-0.00063	-0.00082	-3.13400
D32	0.00680	-0.00002	-0.00010	0.00000	-0.00010	0.00671
D33	-0.01465	0.00007	0.00014	0.00137	0.00151	-0.01314
D34	3.12533	0.00003	0.00025	0.00197	0.00221	3.12754
D35	3.13473	0.00005	0.00017	0.00031	0.00048	3.13521
D36	-0.00848	0.00001	0.00028	0.00091	0.00119	-0.00729
D37	0.03446	-0.00008	-0.00089	-0.00256	-0.00344	0.03101
D38	-3.10153	-0.00003	-0.00109	-0.00325	-0.00433	-3.10587
D39	-3.11444	-0.00011	-0.00088	-0.00049	-0.00136	-3.11579
D40	0.03276	-0.00006	-0.00107	-0.00118	-0.00225	0.03051
D41	1.27739	-0.00011	-0.00218	-0.03137	-0.03355	1.24383
D42	-2.89756	-0.00006	-0.00247	-0.03037	-0.03284	-2.93040
D43	-0.81100	0.00000	-0.00219	-0.03009	-0.03228	-0.84328
D44	-1.85696	-0.00008	-0.00219	-0.03344	-0.03563	-1.89259

This journal is © The Royal Society of Chemistry 2014

D45	0.25128	-0.00002	-0.00248	-0.03244	-0.03492	0.21636
D46	2.33784	0.00003	-0.00220	-0.03215	-0.03435	2.30348
D47	-0.01060	0.00001	0.00042	0.00061	0.00104	-0.00956
D48	3.13259	0.00004	0.00032	0.00002	0.00034	3.13293
D49	3.12575	-0.00003	0.00061	0.00127	0.00187	3.12762
D50	-0.01425	0.00000	0.00050	0.00067	0.00118	-0.01307
D51	-3.13977	-0.00001	-0.00010	-0.00022	-0.00032	-3.14009
D52	0.01456	-0.00003	-0.00050	0.00013	-0.00037	0.01419
D53	0.00729	0.00004	-0.00029	-0.00090	-0.00119	0.00610
D54	-3.12157	0.00002	-0.00069	-0.00054	-0.00123	-3.12281
D55	0.00711	0.00003	-0.00037	-0.00052	-0.00089	0.00621
D56	-3.12950	0.00001	-0.00046	-0.00071	-0.00116	-3.13066
D57	-3.13610	0.00000	-0.00026	0.00008	-0.00019	-3.13629
D58	0.01048	-0.00002	-0.00035	-0.00011	-0.00046	0.01002
D59	0.00092	0.00001	-0.00004	-0.00028	-0.00031	0.00061
D60	3.13938	0.00000	0.00006	-0.00035	-0.00029	3.13908
D61	-3.13555	-0.00001	-0.00012	-0.00047	-0.00059	-3.13614
D62	0.00291	-0.00002	-0.00003	-0.00054	-0.00057	0.00233
D63	-0.00828	0.00003	0.00026	0.00007	0.00033	-0.00795
D64	3.13124	0.00002	0.00037	0.00066	0.00103	3.13227
D65	3.13643	0.00003	0.00017	0.00014	0.00031	3.13673
D66	-0.00724	0.00002	0.00027	0.00074	0.00101	-0.00623
D67	0.00393	-0.00005	-0.00009	0.00054	0.00046	0.00438
D68	3.13295	-0.00003	0.00031	0.00020	0.00051	3.13345
D69	-3.13558	-0.00004	-0.00019	-0.00006	-0.00025	-3.13583
D70	-0.00657	-0.00002	0.00020	-0.00040	-0.00020	-0.00676

This journal is © The Royal Society of Chemistry 2014

Item	Value	Threshold	Converged?
Maximum Force	0.000380	0.000450	YES
RMS Force	0.000101	0.000300	YES
Maximum Displacement	0.070461	0.001800	NO
RMS Displacement	0.009826	0.001200	NO

Predicted change in Energy=-1.105765D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.793021	-5.420126	0.018277
2	6	0	-3.422596	-5.393067	-0.007837
3	6	0	-2.705962	-4.154472	-0.020706
4	6	0	-3.440311	-2.909686	-0.019271
5	6	0	-4.871660	-2.989829	0.013138
6	6	0	-5.524484	-4.198219	0.033813
7	6	0	-1.308028	-4.125765	-0.033112
8	6	0	-2.747926	-1.673191	-0.040232
9	6	0	-1.329802	-1.663257	-0.025177
10	6	0	-0.604083	-2.918126	-0.027591
11	6	0	0.827640	-2.905349	-0.023167
12	1	0	1.347492	-3.861188	-0.030205
13	6	0	1.528800	-1.728852	-0.004950
14	6	0	0.826172	-0.490086	0.010710
15	6	0	-0.546128	-0.459948	-0.001593
16	1	0	-0.755647	-5.063883	-0.040952
17	1	0	-5.326412	-6.367408	0.030726
18	1	0	-2.849432	-6.317929	-0.015025
19	1	0	-5.457278	-2.076768	0.032981
20	1	0	-6.611161	-4.225798	0.063188
21	1	0	2.615978	-1.732546	0.000573
22	1	0	1.385935	0.441895	0.033979
23	1	0	-1.041160	0.504084	0.018839
24	6	0	-3.550083	-0.388835	-0.071671
25	1	0	-4.048725	-0.199865	0.889052
26	1	0	-2.938815	0.485296	-0.296441
27	1	0	-4.330733	-0.429096	-0.838830

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370941	0.000000			
3	C	2.441150	1.431030	0.000000		
4	C	2.851936	2.483471	1.445256	0.000000	
5	C	2.431574	2.806382	2.459225	1.433957	0.000000
6	C	1.424196	2.418125	2.819389	2.450900	1.373613
7	C	3.717955	2.465379	1.398284	2.454725	3.740583

This journal is © The Royal Society of Chemistry 2014

8	C	4.269117	3.780702	2.481713	1.417306	2.499326
9	C	5.109778	4.276865	2.846048	2.451096	3.782330
10	C	4.879478	3.750965	2.438543	2.836253	4.268373
11	C	6.157730	4.924782	3.747887	4.267955	5.700041
12	H	6.335498	5.010079	4.064061	4.881448	6.280047
13	C	7.320618	6.159773	4.880275	5.107508	6.523517
14	C	7.475338	6.487804	5.089664	4.904921	6.222058
15	C	6.529920	5.710496	4.279574	3.791810	5.011062
16	H	4.053492	2.687391	2.152014	3.442158	4.609358
17	H	1.087200	2.139005	3.430232	3.938999	3.408100
18	H	2.141191	1.088089	2.168216	3.459086	3.894413
19	H	3.408738	3.890943	3.448112	2.182805	1.084907
20	H	2.175792	3.396249	3.906752	3.434129	2.134476
21	H	8.275978	7.061435	5.847155	6.169659	7.592472
22	H	8.517219	7.561118	6.154121	5.876103	7.136852
23	H	7.012326	6.359901	4.947249	4.172674	5.184611
24	C	5.183326	5.006263	3.859425	2.523784	2.918720
25	H	5.344469	5.307146	4.274294	2.922045	3.037819
26	H	6.197671	5.905293	4.653783	3.442996	3.988511
27	H	5.085147	5.114321	4.145798	2.760047	2.752418

		6	7	8	9	10
6	C	0.000000				
7	C	4.217609	0.000000			
8	C	3.753735	2.844025	0.000000		
9	C	4.901517	2.462617	1.418239	0.000000	
10	C	5.084560	1.397841	2.479130	1.449610	0.000000
11	C	6.482610	2.459795	3.781954	2.489448	1.431787
12	H	6.880533	2.668669	4.643262	3.463932	2.167491
13	C	7.473158	3.713970	4.277234	2.859426	2.442145
14	C	7.354021	4.216028	3.765171	2.454759	2.818240
15	C	6.225749	3.744288	2.514232	1.436194	2.458998
16	H	4.847346	1.088692	3.932679	3.448790	2.151144
17	H	2.178215	4.601788	5.356239	6.172929	5.848191
18	H	3.413423	2.679895	4.645916	4.896463	4.074360
19	H	2.122516	4.628071	2.740223	4.148546	4.925957
20	H	1.087424	5.304951	4.631532	5.870876	6.148433
21	H	8.505749	4.596352	5.364387	3.946472	3.431499
22	H	8.323734	5.303344	4.644125	3.436625	3.905599
23	H	6.497082	4.637825	2.767140	2.186920	3.450321
24	C	4.291945	4.358089	1.514600	2.560461	3.883062
25	H	4.346968	4.875910	2.174013	3.220228	4.482715
26	H	5.360043	4.898029	2.182005	2.697923	4.136004
27	H	4.048807	4.842654	2.165828	3.345262	4.554262

		11	12	13	14	15
11	C	0.000000				
12	H	1.088083	0.000000			
13	C	1.369708	2.140178	0.000000		
14	C	2.415501	3.411419	1.424245	0.000000	
15	C	2.804940	3.892948	2.432171	1.372686	0.000000
16	H	2.677010	2.422764	4.042576	4.839880	4.608867
17	H	7.061240	7.129225	8.277161	8.508678	7.599357
18	H	5.016635	4.863124	6.342605	6.890173	6.294548

This journal is © The Royal Society of Chemistry 2014

19	H	6.339550	7.035129	6.994839	6.480725	5.170560
20	H	7.555581	7.967548	8.514596	8.322994	7.139359
21	H	2.138734	2.478128	1.087198	2.178810	3.408581
22	H	3.393965	4.303733	2.175792	1.087412	2.132476
23	H	3.888240	4.976310	3.404595	2.115507	1.083897
24	C	5.049718	6.003765	5.253108	4.378201	3.005613
25	H	5.650727	6.585550	5.851993	4.961888	3.623407
26	H	5.075168	6.110256	4.994698	3.901390	2.589474
27	H	5.779788	6.683964	6.059609	5.226769	3.876230

		16	17	18	19	20
16	H	0.000000				
17	H	4.753546	0.000000			
18	H	2.440746	2.477896	0.000000		
19	H	5.570786	4.292636	4.979018	0.000000	
20	H	5.916103	2.497624	4.305083	2.439404	0.000000
21	H	4.739977	9.195891	7.134192	8.080656	9.558259
22	H	5.908094	9.561497	7.977215	7.291998	9.259685
23	H	5.575603	8.098205	7.057681	5.114987	7.307439
24	C	5.446640	6.237721	5.970618	2.549012	4.910262
25	H	5.947094	6.356712	6.299711	2.497928	4.843167
26	H	5.968658	7.264103	6.809629	3.607678	5.984134
27	H	5.907546	6.083671	6.127909	2.178068	4.519838

		21	22	23	24	25
21	H	0.000000				
22	H	2.498462	0.000000			
23	H	4.286899	2.427939	0.000000		
24	C	6.311187	5.006550	2.664618	0.000000	
25	H	6.896141	5.538820	3.209090	1.098791	0.000000
26	H	5.988553	4.337571	1.923759	1.090080	1.762594
27	H	7.117610	5.848138	3.525296	1.095249	1.765687

		26	27
26	H	0.000000	
27	H	1.751494	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.652952	-1.002993	0.016033
2	6	0	-2.454014	-1.667359	-0.009303
3	6	0	-1.212460	-0.955771	-0.015313
4	6	0	-1.222796	0.489428	-0.007660
5	6	0	-2.501092	1.138435	0.023662
6	6	0	-3.672319	0.420908	0.037668
7	6	0	0.011057	-1.632578	-0.026920
8	6	0	-0.003245	1.211406	-0.021784

```
      9          6           0        1.228228    0.508109   -0.006020
     10          6           0        1.226041   -0.941474   -0.014710
     11          6           0        2.470735   -1.649092   -0.009555
     12          1           0        2.440603   -2.736693   -0.021388
     13          6           0        3.667640   -0.983580    0.015186
     14          6           0        3.681676    0.440428    0.037048
     15          6           0        2.509941    1.155370    0.024267
     16          1           0        0.017956   -2.721176   -0.039447
     17          1           0       -4.589797   -1.554604    0.023242
     18          1           0       -2.422487   -2.754927   -0.021098
     19          1           0       -2.549352    2.221994    0.048044
     20          1           0       -4.626116    0.942383    0.066393
     21          1           0        4.606067   -1.532504    0.021194
     22          1           0        4.633540    0.965414    0.065486
     23          1           0        2.565612    2.237541    0.049549
     24          6           0       -0.052265    2.725006   -0.046827
     25          1           0       -0.391614    3.134581    0.914647
     26          1           0        0.915863    3.175178   -0.266706
     27          1           0       -0.745320    3.085348   -0.814550
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3939576      0.4479668
0.3397951
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9755363663 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860644249     A.U. after   10 cycles
             Convg  =    0.8012D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000027698   -0.000285600    0.000051126
      2        6           0.000101462   -0.000077532    0.000041849
      3        6          -0.000143474   -0.000078253   -0.000093568
      4        6           0.000065611   -0.000108692    0.000250168
      5        6          -0.000594145   -0.000039341    0.000073184
      6        6          -0.000230261    0.000200328   -0.000115081
      7        6           0.000193651   -0.000011784    0.000047808
      8        6           0.000641610    0.000429288   -0.000157670
      9        6          -0.000608647    0.000130679   -0.000246036
```

```
     10        6           -0.000084135   -0.000128071   -0.000115001
     11        6            0.000031405   -0.000224706    0.000071005
     12        1            0.000110102    0.000177027   -0.000022721
     13        6            0.000408855   -0.000134848    0.000028463
     14        6           -0.000141538    0.000388687   -0.000094569
     15        6            0.000077877    0.000104533    0.000168894
     16        1           -0.000030868    0.000105465    0.000085174
     17        1            0.000259101    0.000059533   -0.000008359
     18        1           -0.000203381   -0.000013407   -0.000000918
     19        1            0.000125385   -0.000274502   -0.000080411
     20        1            0.000178302    0.000128246   -0.000017742
     21        1           -0.000198308   -0.000206942    0.000017761
     22        1           -0.000218934   -0.000083424   -0.000048367
     23        1            0.000094517   -0.000080323   -0.000016087
     24        6            0.000458528    0.000239804    0.000240202
     25        1           -0.000055156   -0.000077628    0.000018923
     26        1            0.000059138   -0.000011878    0.000123966
     27        1           -0.000268998   -0.000126660   -0.000201994
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000641610 RMS     0.000200535


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000584416 RMS     0.000125382
 Search for a local minimum.
 Step number  39 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   18   21   20   23
22
                                                     25   24   27   26
28
                                                     29   30   31   32
33
                                                     35   34   36   37
38
                                                     39
 DE= -9.67D-06 DEPred=-1.11D-05 R= 8.75D-01
 SS=  1.41D+00  RLast= 8.41D-02 DXNew= 1.4142D-01 2.5227D-01
 Trust test= 8.75D-01 RLast= 8.41D-02 DXMaxT set to 1.41D-01
     Eigenvalues ---    0.00002   0.00191   0.00869   0.01142
0.01603
     Eigenvalues ---    0.01780   0.01785   0.01818   0.01858
0.01892
     Eigenvalues ---    0.01952   0.01975   0.01981   0.02068
0.02094
     Eigenvalues ---    0.02097   0.02144   0.02147   0.02220
0.02224
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02298   0.02343   0.02581   0.06321
0.06899
     Eigenvalues ---    0.10805   0.12103   0.15544   0.15769
0.15982
     Eigenvalues ---    0.16000   0.16002   0.16002   0.16012
0.16173
     Eigenvalues ---    0.16517   0.18541   0.21075   0.22008
0.22577
     Eigenvalues ---    0.22772   0.23163   0.23953   0.24579
0.24604
     Eigenvalues ---    0.25228   0.27755   0.30232   0.32411
0.33397
     Eigenvalues ---    0.33590   0.33629   0.33634   0.33682
0.33683
     Eigenvalues ---    0.33963   0.34124   0.34994   0.36076
0.37082
     Eigenvalues ---    0.37506   0.38078   0.38242   0.39763
0.40221
     Eigenvalues ---    0.40765   0.40962   0.43406   0.44530
0.45250
     Eigenvalues ---    0.49109   0.49853   0.50566   0.51262
0.61017
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   2.09D-05 Eigenvector:
```

This journal is © The Royal Society of Chemistry 2014

```
                         D41       D42       D44       D43       D45
   1                   0.42170   0.41859   0.39750   0.39446
0.39440
                         D46       D28       D39       D26       D40
   1                   0.37026  -0.06697   0.05866  -0.05845
0.05660
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    39   38   37   36
 RFO step:  Lambda=-9.22924804D-06.
 DIIS coeffs:      2.85235     -2.21605      2.33005     -1.96635
 Maximum step size (   0.141) exceeded in Quadratic search.
    -- Step size scaled by   0.193
 Iteration  1 RMS(Cart)=  0.01746549 RMS(Int)=  0.00042160
 Iteration  2 RMS(Cart)=  0.00043995 RMS(Int)=  0.00000216
 Iteration  3 RMS(Cart)=  0.00000024 RMS(Int)=  0.00000215
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59070  -0.00013   0.00002  -0.00012  -0.00010
2.59061
    R2        2.69134   0.00024  -0.00005   0.00059   0.00055
2.69189
    R3        2.05451  -0.00018   0.00018  -0.00070  -0.00051
2.05400
    R4        2.70426   0.00007   0.00004   0.00019   0.00023
2.70449
    R5        2.05619  -0.00010   0.00002  -0.00064  -0.00062
2.05557
    R6        2.73114   0.00014  -0.00040   0.00004  -0.00036
2.73078
    R7        2.64237   0.00012   0.00005   0.00032   0.00038
2.64275
    R8        2.70979   0.00042  -0.00047   0.00059   0.00012
2.70991
    R9        2.67832   0.00058  -0.00025   0.00114   0.00088
2.67921
   R10        2.59575  -0.00012   0.00025   0.00026   0.00052
2.59627
   R11        2.05018  -0.00030   0.00034  -0.00073  -0.00039
2.04979
   R12        2.05493  -0.00018   0.00004  -0.00099  -0.00095
2.05398
   R13        2.64154  -0.00009   0.00025  -0.00001   0.00024
2.64178
   R14        2.05733  -0.00011   0.00002  -0.00068  -0.00065
2.05668
   R15        2.68008  -0.00048   0.00056   0.00082   0.00137
2.68146
   R16        2.86218  -0.00009  -0.00017  -0.00015  -0.00032
2.86186
   R17        2.73937   0.00017   0.00007   0.00153   0.00160
2.74096
```

This journal is © The Royal Society of Chemistry 2014

R18	2.71401	0.00004	-0.00006	0.00100	0.00094
2.71495					
R19	2.70568	0.00013	0.00005	0.00047	0.00052
2.70620					
R20	2.05618	-0.00010	0.00002	-0.00065	-0.00063
2.05555					
R21	2.58837	-0.00003	-0.00017	-0.00044	-0.00062
2.58776					
R22	2.69143	0.00037	-0.00016	0.00070	0.00054
2.69198					
R23	2.05451	-0.00020	0.00020	-0.00072	-0.00051
2.05399					
R24	2.59400	-0.00014	0.00016	-0.00006	0.00010
2.59410					
R25	2.05491	-0.00018	0.00004	-0.00101	-0.00097
2.05394					
R26	2.04827	-0.00011	0.00015	-0.00098	-0.00083
2.04744					
R27	2.07641	0.00003	-0.00033	0.00013	-0.00019
2.07622					
R28	2.05995	0.00000	-0.00038	-0.00074	-0.00112
2.05883					
R29	2.06972	0.00034	0.00008	0.00163	0.00170
2.07142					
A1	2.09056	0.00001	0.00028	0.00043	0.00071
2.09127					
A2	2.10347	-0.00021	0.00045	-0.00138	-0.00094
2.10253					
A3	2.08914	0.00020	-0.00073	0.00096	0.00024
2.08938					
A4	2.11513	0.00004	-0.00035	-0.00028	-0.00064
2.11449					
A5	2.10588	-0.00021	0.00074	-0.00082	-0.00007
2.10581					
A6	2.06217	0.00016	-0.00039	0.00111	0.00072
2.06288					
A7	2.08404	0.00007	-0.00010	0.00003	-0.00006
2.08398					
A8	2.11590	-0.00001	0.00026	0.00038	0.00064
2.11654					
A9	2.08324	-0.00006	-0.00016	-0.00041	-0.00057
2.08267					
A10	2.04775	-0.00018	0.00067	0.00044	0.00112
2.04886					
A11	2.09807	-0.00009	0.00033	0.00051	0.00084
2.09890					
A12	2.13735	0.00027	-0.00102	-0.00093	-0.00195
2.13540					
A13	2.12222	0.00006	-0.00053	-0.00051	-0.00105
2.12117					
A14	2.08539	0.00001	-0.00014	-0.00056	-0.00070
2.08469					

This journal is © The Royal Society of Chemistry 2014

A15	2.07551	-0.00007	0.00069	0.00111	0.00179
2.07730					
A16	2.10657	0.00000	0.00003	-0.00005	-0.00002
2.10655					
A17	2.08493	0.00013	-0.00044	0.00051	0.00007
2.08499					
A18	2.09169	-0.00012	0.00041	-0.00046	-0.00004
2.09164					
A19	2.11902	0.00003	-0.00004	0.00025	0.00021
2.11923					
A20	2.08246	0.00001	0.00001	-0.00006	-0.00004
2.08241					
A21	2.08169	-0.00004	0.00003	-0.00019	-0.00016
2.08153					
A22	2.08798	0.00001	0.00014	0.00020	0.00034
2.08832					
A23	2.07303	0.00017	-0.00180	-0.00431	-0.00611
2.06691					
A24	2.12217	-0.00018	0.00167	0.00409	0.00576
2.12793					
A25	2.08807	0.00007	-0.00051	-0.00108	-0.00160
2.08646					
A26	2.15515	-0.00005	0.00036	0.00195	0.00232
2.15747					
A27	2.03996	-0.00002	0.00016	-0.00087	-0.00072
2.03924					
A28	2.08951	0.00004	0.00027	0.00069	0.00096
2.09047					
A29	2.10749	-0.00004	-0.00034	-0.00110	-0.00144
2.10605					
A30	2.08619	0.00000	0.00007	0.00041	0.00048
2.08667					
A31	2.05996	0.00019	-0.00059	0.00090	0.00031
2.06027					
A32	2.11717	0.00000	-0.00020	-0.00001	-0.00022
2.11695					
A33	2.10605	-0.00019	0.00080	-0.00089	-0.00009
2.10596					
A34	2.08827	-0.00004	0.00015	0.00000	0.00015
2.08842					
A35	2.10487	-0.00019	0.00055	-0.00118	-0.00064
2.10424					
A36	2.09004	0.00023	-0.00070	0.00119	0.00048
2.09052					
A37	2.10853	0.00000	0.00018	0.00028	0.00046
2.10900					
A38	2.08487	0.00015	-0.00044	0.00050	0.00006
2.08493					
A39	2.08978	-0.00015	0.00026	-0.00078	-0.00052
2.08926					
A40	2.12617	0.00006	-0.00033	0.00021	-0.00013
2.12604					

This journal is © The Royal Society of Chemistry 2014

A41	2.09012	0.00002	0.00007	0.00041	0.00047
2.09059					
A42	2.06683	-0.00008	0.00029	-0.00059	-0.00031
2.06653					
A43	1.94769	-0.00008	-0.00035	-0.00111	-0.00146
1.94622					
A44	1.96849	0.00000	0.00082	0.00123	0.00205
1.97054					
A45	1.93998	-0.00010	-0.00070	-0.00366	-0.00437
1.93562					
A46	1.87219	0.00003	-0.00076	0.00103	0.00027
1.87247					
A47	1.87056	0.00001	0.00010	0.00018	0.00026
1.87082					
A48	1.85952	0.00014	0.00091	0.00259	0.00350
1.86303					
D1	-0.00065	0.00000	-0.00009	0.00026	0.00017	-
0.00048					
D2	3.13631	0.00003	-0.00028	0.00163	0.00134
3.13765					
D3	-3.13851	-0.00003	0.00025	-0.00134	-0.00110	-
3.13961					
D4	-0.00155	0.00000	0.00006	0.00002	0.00008	-
0.00147					
D5	0.00828	-0.00005	0.00002	-0.00281	-0.00280
0.00548					
D6	-3.13243	-0.00003	-0.00011	-0.00248	-0.00259	-
3.13502					
D7	-3.13701	-0.00002	-0.00032	-0.00122	-0.00154	-
3.13856					
D8	0.00546	0.00000	-0.00044	-0.00089	-0.00134
0.00413					
D9	-0.01062	0.00005	0.00004	0.00326	0.00331	-
0.00731					
D10	3.12969	0.00004	-0.00012	0.00302	0.00290
3.13259					
D11	3.13550	0.00002	0.00022	0.00194	0.00216
3.13766					
D12	-0.00738	0.00000	0.00006	0.00170	0.00175	-
0.00563					
D13	0.01405	-0.00005	0.00009	-0.00419	-0.00410
0.00995					
D14	-3.13478	-0.00001	-0.00095	-0.00136	-0.00232	-
3.13710					
D15	-3.12628	-0.00004	0.00025	-0.00395	-0.00370	-
3.12999					
D16	0.00807	0.00000	-0.00079	-0.00113	-0.00192
0.00615					
D17	-3.12641	-0.00006	0.00078	-0.00271	-0.00193	-
3.12834					
D18	0.00841	-0.00004	0.00044	-0.00163	-0.00119
0.00723					

This journal is © The Royal Society of Chemistry 2014

D19	0.01390	-0.00007	0.00061	-0.00295	-0.00234	0.01156
D20	-3.13446	-0.00006	0.00028	-0.00187	-0.00159	-3.13606
D21	-0.00679	0.00000	-0.00016	0.00175	0.00159	-0.00520
D22	3.12279	0.00006	0.00054	0.00597	0.00650	3.12930
D23	-3.14097	-0.00004	0.00090	-0.00114	-0.00025	-3.14122
D24	-0.01139	0.00002	0.00160	0.00307	0.00467	-0.00672
D25	-0.03039	0.00006	0.00128	0.00486	0.00614	-0.02425
D26	3.11627	0.00011	0.00060	0.00808	0.00868	3.12495
D27	3.10358	0.00011	0.00019	0.00783	0.00802	3.11161
D28	-0.03294	0.00016	-0.00049	0.01106	0.01057	-0.02238
D29	-0.00435	0.00005	0.00011	0.00175	0.00186	-0.00249
D30	3.13636	0.00003	0.00024	0.00141	0.00165	3.13801
D31	-3.13400	-0.00001	-0.00058	-0.00244	-0.00302	-3.13702
D32	0.00671	-0.00003	-0.00045	-0.00277	-0.00322	0.00348
D33	-0.01314	0.00006	-0.00091	0.00320	0.00229	-0.01085
D34	3.12754	0.00002	-0.00036	0.00179	0.00143	3.12897
D35	3.13521	0.00005	-0.00057	0.00212	0.00154	3.13676
D36	-0.00729	0.00001	-0.00003	0.00071	0.00068	-0.00661
D37	0.03101	-0.00007	-0.00158	-0.00461	-0.00618	0.02483
D38	-3.10587	-0.00002	-0.00250	-0.00357	-0.00607	-3.11193
D39	-3.11579	-0.00012	-0.00089	-0.00796	-0.00885	-3.12465
D40	0.03051	-0.00007	-0.00181	-0.00692	-0.00874	0.02177
D41	1.24383	-0.00009	-0.02234	-0.03667	-0.05901	1.18482
D42	-2.93040	-0.00011	-0.02300	-0.03526	-0.05826	-2.98866
D43	-0.84328	0.00001	-0.02176	-0.03368	-0.05544	-0.89872
D44	-1.89259	-0.00004	-0.02303	-0.03336	-0.05639	-1.94898

This journal is © The Royal Society of Chemistry 2014

D45	0.21636	-0.00006	-0.02368	-0.03195	-0.05564	0.16073
D46	2.30348	0.00006	-0.02244	-0.03037	-0.05282	2.25067
D47	-0.00956	0.00001	0.00139	0.00062	0.00201	-0.00755
D48	3.13293	0.00005	0.00085	0.00202	0.00287	3.13580
D49	3.12762	-0.00004	0.00225	-0.00034	0.00191	3.12953
D50	-0.01307	0.00000	0.00171	0.00106	0.00277	-0.01030
D51	-3.14009	0.00000	-0.00040	-0.00008	-0.00047	-3.14056
D52	0.01419	-0.00005	-0.00177	-0.00279	-0.00456	0.00964
D53	0.00610	0.00005	-0.00129	0.00093	-0.00036	0.00574
D54	-3.12281	0.00000	-0.00266	-0.00178	-0.00444	-3.12725
D55	0.00621	0.00003	-0.00151	0.00030	-0.00121	0.00501
D56	-3.13066	0.00001	-0.00159	-0.00028	-0.00187	-3.13253
D57	-3.13629	-0.00001	-0.00096	-0.00111	-0.00207	-3.13835
D58	0.01002	-0.00003	-0.00104	-0.00169	-0.00273	0.00729
D59	0.00061	0.00001	-0.00015	0.00033	0.00018	0.00079
D60	3.13908	0.00002	0.00026	0.00072	0.00098	3.14006
D61	-3.13614	-0.00001	-0.00023	-0.00027	-0.00050	-3.13665
D62	0.00233	-0.00001	0.00018	0.00012	0.00030	0.00263
D63	-0.00795	0.00004	0.00062	0.00170	0.00232	-0.00563
D64	3.13227	0.00001	0.00085	0.00093	0.00178	3.13405
D65	3.13673	0.00003	0.00021	0.00132	0.00153	3.13826
D66	-0.00623	0.00001	0.00044	0.00055	0.00099	-0.00524
D67	0.00438	-0.00007	0.00014	-0.00235	-0.00221	0.00218
D68	3.13345	-0.00002	0.00150	0.00033	0.00183	3.13528
D69	-3.13583	-0.00005	-0.00010	-0.00158	-0.00167	-3.13751
D70	-0.00676	0.00000	0.00126	0.00110	0.00236	-0.00440

This journal is © The Royal Society of Chemistry 2014

```
         Item               Value     Threshold  Converged?
 Maximum Force            0.000584     0.000450     NO
 RMS     Force            0.000125     0.000300     YES
 Maximum Displacement     0.131314     0.001800     NO
 RMS     Displacement     0.017463     0.001200     NO
 Predicted change in Energy=-2.364469D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792927   -5.417559    0.019525
      2          6           0       -3.422447   -5.392024   -0.002137
      3          6           0       -2.705190   -4.153665   -0.016739
      4          6           0       -3.438967   -2.908762   -0.017698
      5          6           0       -4.870618   -2.986774    0.008962
      6          6           0       -5.524157   -4.195109    0.028384
      7          6           0       -1.307054   -4.124705   -0.028083
      8          6           0       -2.746868   -1.671552   -0.037557
      9          6           0       -1.327986   -1.660647   -0.026616
     10          6           0       -0.603046   -2.916944   -0.026552
     11          6           0        0.828969   -2.906209   -0.022733
     12          1           0        1.347576   -3.862367   -0.025882
     13          6           0        1.531408   -1.730777   -0.010595
     14          6           0        0.830351   -0.490733   -0.000561
     15          6           0       -0.541973   -0.458162   -0.009538
     16          1           0       -0.754694   -5.062455   -0.032612
     17          1           0       -5.326354   -6.364504    0.032312
     18          1           0       -2.850500   -6.317277   -0.005448
     19          1           0       -5.454304   -2.072582    0.020681
     20          1           0       -6.610489   -4.222148    0.051789
     21          1           0        2.618311   -1.736458   -0.006387
     22          1           0        1.391104    0.440193    0.016195
     23          1           0       -1.034696    0.506673    0.004644
     24          6           0       -3.557333   -0.392435   -0.059957
     25          1           0       -4.099149   -0.242238    0.883968
     26          1           0       -2.946170    0.493889   -0.226953
     27          1           0       -4.304226   -0.416685   -0.861896
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1          2          3          4          5
    1  C    0.000000
    2  C    1.370889   0.000000
    3  C    2.440776   1.431155   0.000000
    4  C    2.851079   2.483366   1.445065   0.000000
    5  C    2.432049   2.807588   2.459953   1.434022   0.000000
    6  C    1.424486   2.418827   2.819632   2.450475   1.373886
    7  C    3.718205   2.466102   1.398483   2.454319   3.741022
```

This journal is © The Royal Society of Chemistry 2014

8	C	4.268745	3.781478	2.482550	1.417775	2.498457
9	C	5.111001	4.279082	2.848145	2.452369	3.782872
10	C	4.879580	3.751752	2.438973	2.835948	4.268291
11	C	6.157465	4.924859	3.747861	4.267940	5.700244
12	H	6.334545	5.009345	4.063232	4.880618	6.279635
13	C	7.320552	6.159991	4.880491	5.108066	6.524098
14	C	7.476314	6.489140	5.090912	4.906550	6.223452
15	C	6.532003	5.713158	4.282091	3.794480	5.013121
16	H	4.054151	2.688205	2.151880	3.441503	4.609882
17	H	1.086929	2.138169	3.429390	3.937878	3.408416
18	H	2.140827	1.087762	2.168515	3.458962	3.895296
19	H	3.409734	3.892000	3.448178	2.182258	1.084700
20	H	2.175679	3.396341	3.906500	3.433419	2.134276
21	H	8.275121	7.060732	5.846594	6.169688	7.592601
22	H	8.517951	7.562100	6.155017	5.877604	7.138159
23	H	7.015771	6.363649	4.950733	4.176867	5.188303
24	C	5.175411	5.001743	3.856795	2.519464	2.908619
25	H	5.292686	5.269099	4.248959	2.891226	2.982160
26	H	6.198102	5.909429	4.658542	3.444513	3.984240
27	H	5.101418	5.125497	4.151653	2.769799	2.772102

		6	7	8	9	10
6	C	0.000000				
7	C	4.218069	0.000000			
8	C	3.753135	2.844489	0.000000		
9	C	4.902486	2.464148	1.418966	0.000000	
10	C	5.084689	1.397969	2.479334	1.450456	0.000000
11	C	6.482753	2.459136	3.783015	2.490762	1.432059
12	H	6.879999	2.667562	4.643736	3.464997	2.167660
13	C	7.473651	3.713228	4.278771	2.860299	2.441954
14	C	7.355475	4.216042	3.767253	2.455157	2.818120
15	C	6.228030	3.745561	2.516875	1.436690	2.459599
16	H	4.848070	1.088346	3.932812	3.449783	2.150873
17	H	2.178398	4.601643	5.355598	6.173872	5.847972
18	H	3.413676	2.681438	4.646992	4.899255	4.075998
19	H	2.123690	4.627448	2.737595	4.147098	4.924417
20	H	1.086921	5.304932	4.630453	5.871310	6.148095
21	H	8.505643	4.594854	5.365662	3.947077	3.430903
22	H	8.325083	5.302858	4.645983	3.436395	3.904974
23	H	6.500968	4.639495	2.770916	2.187298	3.450862
24	C	4.282118	4.358281	1.514429	2.565046	3.886139
25	H	4.288106	4.868386	2.172742	3.243515	4.495091
26	H	5.357043	4.904861	2.182825	2.701977	4.142967
27	H	4.069068	4.840217	2.163236	3.332137	4.543989

		11	12	13	14	15
11	C	0.000000				
12	H	1.087751	0.000000			
13	C	1.369383	2.139557	0.000000		
14	C	2.415578	3.411169	1.424532	0.000000	
15	C	2.805814	3.893492	2.432789	1.372740	0.000000
16	H	2.675347	2.420702	4.040647	4.838806	4.609262
17	H	7.060512	7.127792	8.276604	8.509247	7.601113
18	H	5.017387	4.863213	6.343274	6.891828	6.297503

This journal is © The Royal Society of Chemistry 2014

19	H	6.338480	7.033568	6.994139	6.480709	5.170905
20	H	7.555315	7.966573	8.514771	8.324200	7.141305
21	H	2.137833	2.476820	1.086926	2.179144	3.409025
22	H	3.393511	4.302986	2.175664	1.086898	2.131781
23	H	3.888671	4.976411	3.404601	2.115005	1.083459
24	C	5.055698	6.008304	5.262023	4.389186	3.016497
25	H	5.674962	6.603028	5.892298	5.014391	3.674027
26	H	5.084687	6.119939	5.004464	3.909328	2.594963
27	H	5.766421	6.671920	6.042035	5.206848	3.857821

		16	17	18	19	20
16	H	0.000000				
17	H	4.753906	0.000000			
18	H	2.442891	2.476592	0.000000		
19	H	5.570324	4.293844	4.979750	0.000000	
20	H	5.916382	2.497813	4.304691	2.440977	0.000000
21	H	4.737100	9.194456	7.133849	8.079655	9.557866
22	H	5.906434	9.561820	7.978412	7.292027	9.260895
23	H	5.576288	8.101369	7.061412	5.117202	7.311187
24	C	5.446524	6.229250	5.967105	2.535330	4.899077
25	H	5.938013	6.301864	6.265483	2.435542	4.779020
26	H	5.976060	7.264299	6.815438	3.597059	5.978791
27	H	5.905088	6.100893	6.137084	2.200821	4.542600

		21	22	23	24	25
21	H	0.000000				
22	H	2.498871	0.000000			
23	H	4.286749	2.426738	0.000000		
24	C	6.320431	5.018574	2.678855	0.000000	
25	H	6.938999	5.600145	3.274898	1.098689	0.000000
26	H	5.998879	4.344415	1.925496	1.089485	1.762212
27	H	7.098959	5.825982	3.506182	1.096150	1.766502

		26	27
26	H	0.000000	
27	H	1.754028	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.651146	-1.005934	0.013958
2	6	0	-2.452028	-1.670053	-0.006019
3	6	0	-1.210998	-0.957306	-0.012505
4	6	0	-1.222717	0.487701	-0.006936
5	6	0	-2.501081	1.137007	0.017660
6	6	0	-3.671942	0.418318	0.029215
7	6	0	0.013734	-1.632356	-0.022113
8	6	0	-0.004017	1.212075	-0.018716

```
      9          6           0        1.229542    0.510907   -0.006122
     10          6           0        1.227910   -0.939533   -0.012663
     11          6           0        2.472779   -1.647392   -0.007178
     12          1           0        2.442865   -2.734700   -0.015392
     13          6           0        3.669366   -0.981814    0.012686
     14          6           0        3.683492    0.442551    0.029256
     15          6           0        2.511996    1.158026    0.018935
     16          1           0        0.022258   -2.720628   -0.031560
     17          1           0       -4.587119   -1.558496    0.020557
     18          1           0       -2.420296   -2.757321   -0.014151
     19          1           0       -2.548546    2.220543    0.034122
     20          1           0       -4.625872    0.938828    0.051244
     21          1           0        4.607295   -1.531057    0.018077
     22          1           0        4.634979    0.967429    0.052135
     23          1           0        2.568617    2.239832    0.038261
     24          6           0       -0.064896    2.725198   -0.034471
     25          1           0       -0.462368    3.122242    0.909716
     26          1           0        0.908610    3.187061   -0.195547
     27          1           0       -0.720381    3.081891   -0.837375
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3937097      0.4478532
0.3396919
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.8829894687 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860654124     A.U. after   11 cycles
             Convg  =    0.5951D-08             -V/T =  2.0100
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000132363   -0.000055834    0.000026343
      2        6           0.000080834    0.000363793   -0.000004828
      3        6          -0.000112801   -0.000072851   -0.000062101
      4        6           0.000307482    0.000032533    0.000122026
      5        6          -0.000313329   -0.000590892   -0.000079730
      6        6           0.000222653    0.000274145   -0.000034645
      7        6          -0.000045005    0.000344801    0.000068561
      8        6           0.000927631   -0.000017415    0.000413388
      9        6          -0.000936533   -0.000107454   -0.000138550
```

```
     10        6           -0.000170630   -0.000094092   -0.000086634
     11        6           -0.000380628   -0.000017121    0.000027710
     12        1            0.000171385   -0.000031829   -0.000045824
     13        6            0.000287873    0.000129760   -0.000005337
     14        6           -0.000343817    0.000036500   -0.000016680
     15        6           -0.000023517   -0.000464772   -0.000025873
     16        1            0.000091852   -0.000084593    0.000078141
     17        1            0.000084141   -0.000065558    0.000007213
     18        1           -0.000060157   -0.000173331   -0.000012983
     19        1           -0.000076217   -0.000342043    0.000018501
     20        1           -0.000164485    0.000088278   -0.000016399
     21        1           -0.000008159   -0.000112192    0.000032638
     22        1           -0.000013611    0.000199636   -0.000040837
     23        1           -0.000169165    0.000203164   -0.000006138
     24        6            0.000630438    0.000039267   -0.000162057
     25        1            0.000069512   -0.000077229   -0.000121066
     26        1            0.000189308    0.000283708    0.000062827
     27        1           -0.000112694    0.000311622    0.000002335
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000936533 RMS     0.000239068


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.001552806 RMS     0.000284599
 Search for a local minimum.
 Step number  40 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   28   29   30   31
32
                                                     33   35   34   36
37
                                                     38   39   40
 DE= -9.88D-06 DEPred=-2.36D-05 R= 4.18D-01
 Trust test= 4.18D-01 RLast= 1.41D-01 DXMaxT set to 1.41D-01
     Eigenvalues ---    0.00001   0.00343   0.00929   0.01591
0.01618
     Eigenvalues ---    0.01777   0.01798   0.01813   0.01831
0.01942
     Eigenvalues ---    0.01971   0.01977   0.01987   0.02069
0.02095
     Eigenvalues ---    0.02107   0.02145   0.02148   0.02218
0.02227
     Eigenvalues ---    0.02309   0.02344   0.05186   0.06656
0.07513
     Eigenvalues ---    0.10905   0.14602   0.15452   0.15763
0.15967
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.15999   0.16000   0.16002   0.16014
0.16074
     Eigenvalues ---    0.16447   0.17538   0.21836   0.22016
0.22565
     Eigenvalues ---    0.22674   0.22977   0.24186   0.24596
0.25228
     Eigenvalues ---    0.25394   0.27549   0.31488   0.32937
0.33090
     Eigenvalues ---    0.33590   0.33630   0.33634   0.33682
0.33684
     Eigenvalues ---    0.33965   0.34274   0.34803   0.36259
0.37439
     Eigenvalues ---    0.37489   0.38062   0.38395   0.39742
0.40316
     Eigenvalues ---    0.40717   0.41007   0.43666   0.44674
0.46246
     Eigenvalues ---    0.49315   0.49833   0.51150   0.51450
0.59350
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   6.09D-06 Eigenvector:
                          D45       D44       D46       D42       D41
   1                    0.41956   0.41529   0.40320   0.40111
0.39684
                          D43       D38       D27       D37       D25
```

This journal is © The Royal Society of Chemistry 2014

```
   1                    0.38476   0.05725  -0.04581   0.04228  -
0.04105
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    40   39   38   37
36
 RFO step:  Lambda=-2.11780177D-05.
 DIIS coeffs:      0.56845      0.20016      1.70362     -0.13901
-1.33321
 Maximum step size (   0.141) exceeded in Quadratic search.
    -- Step size scaled by   0.372
 Iteration  1 RMS(Cart)=  0.01705181 RMS(Int)=  0.00042571
 Iteration  2 RMS(Cart)=  0.00044135 RMS(Int)=  0.00000555
 Iteration  3 RMS(Cart)=  0.00000025 RMS(Int)=  0.00000555
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                   (DIIS)     (GDIIS)  (Total)
    R1        2.59061  -0.00005   0.00003  -0.00009  -0.00007
2.59054
    R2        2.69189  -0.00008  -0.00016   0.00044   0.00028
2.69217
    R3        2.05400   0.00002   0.00016  -0.00018  -0.00002
2.05398
    R4        2.70449  -0.00006   0.00004  -0.00013  -0.00009
2.70440
    R5        2.05557   0.00012   0.00005   0.00021   0.00026
2.05583
    R6        2.73078   0.00009   0.00013  -0.00126  -0.00114
2.72964
    R7        2.64275   0.00001  -0.00016   0.00088   0.00072
2.64347
    R8        2.70991   0.00046  -0.00027   0.00020  -0.00007
2.70984
    R9        2.67921   0.00062  -0.00035   0.00108   0.00073
2.67993
   R10        2.59627  -0.00033   0.00007  -0.00006   0.00002
2.59628
   R11        2.04979  -0.00025   0.00018  -0.00015   0.00003
2.04982
   R12        2.05398   0.00016   0.00016  -0.00001   0.00015
2.05413
   R13        2.64178  -0.00031   0.00014  -0.00030  -0.00016
2.64162
   R14        2.05668   0.00012   0.00007   0.00009   0.00016
2.05683
   R15        2.68146  -0.00155   0.00040  -0.00169  -0.00129
2.68016
   R16        2.86186   0.00006  -0.00031  -0.00328  -0.00359
2.85827
   R17        2.74096  -0.00039  -0.00033   0.00013  -0.00020
2.74076
   R18        2.71495  -0.00042  -0.00029   0.00034   0.00005
2.71500
```

This journal is © The Royal Society of Chemistry 2014

R19	2.70620	0.00000	-0.00012	0.00046	0.00034
2.70654					
R20	2.05555	0.00011	0.00006	0.00019	0.00024
2.05580					
R21	2.58776	0.00026	0.00009	-0.00039	-0.00030
2.58746					
R22	2.69198	0.00018	-0.00031	0.00108	0.00077
2.69275					
R23	2.05399	-0.00001	0.00018	-0.00024	-0.00007
2.05393					
R24	2.59410	-0.00028	0.00018	-0.00046	-0.00028
2.59382					
R25	2.05394	0.00016	0.00017	-0.00002	0.00014
2.05408					
R26	2.04744	0.00026	0.00016	0.00013	0.00029
2.04773					
R27	2.07622	-0.00015	-0.00010	0.00014	0.00004
2.07627					
R28	2.05883	0.00033	0.00034	-0.00030	0.00004
2.05887					
R29	2.07142	0.00007	-0.00027	0.00159	0.00132
2.07274					
A1	2.09127	-0.00011	-0.00010	-0.00077	-0.00087
2.09039					
A2	2.10253	-0.00005	0.00072	0.00023	0.00094
2.10348					
A3	2.08938	0.00016	-0.00062	0.00055	-0.00007
2.08931					
A4	2.11449	0.00014	-0.00007	0.00018	0.00011
2.11460					
A5	2.10581	-0.00022	0.00069	0.00040	0.00109
2.10689					
A6	2.06288	0.00007	-0.00062	-0.00057	-0.00119
2.06170					
A7	2.08398	0.00011	0.00014	0.00074	0.00087
2.08485					
A8	2.11654	-0.00010	-0.00031	-0.00025	-0.00055
2.11598					
A9	2.08267	-0.00001	0.00018	-0.00049	-0.00032
2.08235					
A10	2.04886	-0.00044	-0.00013	-0.00058	-0.00071
2.04816					
A11	2.09890	-0.00033	-0.00010	0.00079	0.00068
2.09958					
A12	2.13540	0.00077	0.00023	-0.00021	0.00003
2.13543					
A13	2.12117	0.00029	0.00002	0.00022	0.00024
2.12141					
A14	2.08469	0.00011	0.00036	0.00041	0.00077
2.08545					
A15	2.07730	-0.00040	-0.00036	-0.00062	-0.00099
2.07632					

This journal is © The Royal Society of Chemistry 2014

A16	2.10655	0.00000	0.00016	0.00022	0.00038
2.10693					
A17	2.08499	0.00009	-0.00041	0.00065	0.00024
2.08523					
A18	2.09164	-0.00010	0.00025	-0.00088	-0.00063
2.09102					
A19	2.11923	-0.00005	0.00000	-0.00019	-0.00020
2.11903					
A20	2.08241	0.00006	-0.00005	0.00030	0.00026
2.08267					
A21	2.08153	-0.00001	0.00004	-0.00011	-0.00006
2.08147					
A22	2.08832	0.00000	0.00005	-0.00060	-0.00058
2.08774					
A23	2.06691	0.00155	0.00095	-0.00172	-0.00076
2.06615					
A24	2.12793	-0.00155	-0.00099	0.00231	0.00133
2.12926					
A25	2.08646	0.00051	0.00016	0.00043	0.00057
2.08704					
A26	2.15747	-0.00078	-0.00034	0.00060	0.00028
2.15774					
A27	2.03924	0.00027	0.00019	-0.00103	-0.00084
2.03840					
A28	2.09047	-0.00011	-0.00011	0.00012	0.00000
2.09047					
A29	2.10605	0.00029	0.00003	-0.00069	-0.00065
2.10540					
A30	2.08667	-0.00017	0.00008	0.00057	0.00065
2.08732					
A31	2.06027	0.00013	-0.00057	-0.00095	-0.00152
2.05875					
A32	2.11695	0.00002	-0.00014	0.00043	0.00028
2.11723					
A33	2.10596	-0.00015	0.00072	0.00053	0.00125
2.10721					
A34	2.08842	-0.00011	0.00003	-0.00098	-0.00096
2.08747					
A35	2.10424	-0.00006	0.00066	0.00034	0.00101
2.10524					
A36	2.09052	0.00017	-0.00069	0.00064	-0.00005
2.09048					
A37	2.10900	-0.00013	0.00009	0.00042	0.00051
2.10951					
A38	2.08493	0.00018	-0.00041	0.00083	0.00043
2.08536					
A39	2.08926	-0.00006	0.00032	-0.00126	-0.00094
2.08832					
A40	2.12604	0.00012	-0.00020	0.00060	0.00039
2.12643					
A41	2.09059	-0.00012	0.00004	0.00053	0.00056
2.09115					

This journal is © The Royal Society of Chemistry 2014

A42	2.06653	0.00000	0.00019	-0.00111	-0.00093	2.06560
A43	1.94622	-0.00018	-0.00072	0.00033	-0.00039	1.94583
A44	1.97054	-0.00006	0.00010	0.00482	0.00491	1.97545
A45	1.93562	0.00051	0.00175	0.00122	0.00297	1.93859
A46	1.87247	-0.00001	-0.00108	-0.00304	-0.00412	1.86835
A47	1.87082	-0.00013	0.00005	-0.00365	-0.00359	1.86723
A48	1.86303	-0.00015	-0.00016	-0.00024	-0.00042	1.86261
D1	-0.00048	0.00000	0.00000	-0.00059	-0.00058	-0.00106
D2	3.13765	0.00002	0.00022	0.00057	0.00079	3.13844
D3	-3.13961	-0.00001	0.00012	-0.00172	-0.00161	-3.14122
D4	-0.00147	0.00001	0.00033	-0.00056	-0.00024	-0.00171
D5	0.00548	-0.00002	-0.00067	-0.00165	-0.00232	0.00316
D6	-3.13502	-0.00002	-0.00123	-0.00037	-0.00160	-3.13662
D7	-3.13856	-0.00001	-0.00078	-0.00052	-0.00131	-3.13986
D8	0.00413	0.00000	-0.00134	0.00076	-0.00058	0.00355
D9	-0.00731	0.00002	0.00085	0.00198	0.00284	-0.00447
D10	3.13259	0.00002	0.00098	0.00133	0.00230	3.13489
D11	3.13766	0.00000	0.00064	0.00085	0.00149	3.13915
D12	-0.00563	0.00000	0.00077	0.00019	0.00096	-0.00466
D13	0.00995	-0.00003	-0.00103	-0.00119	-0.00221	0.00773
D14	-3.13710	0.00000	-0.00105	-0.00117	-0.00222	-3.13932
D15	-3.12999	-0.00003	-0.00115	-0.00054	-0.00169	-3.13168
D16	0.00615	0.00000	-0.00117	-0.00053	-0.00170	0.00445
D17	-3.12834	-0.00008	-0.00130	-0.00155	-0.00285	-3.13119
D18	0.00723	-0.00004	-0.00159	-0.00028	-0.00187	0.00536
D19	0.01156	-0.00008	-0.00117	-0.00221	-0.00338	0.00818

This journal is © The Royal Society of Chemistry 2014

D20	-3.13606	-0.00004	-0.00146	-0.00094	-0.00240	-3.13846
D21	-0.00520	0.00001	0.00039	-0.00100	-0.00062	-0.00582
D22	3.12930	0.00001	0.00144	0.00156	0.00300	3.13230
D23	-3.14122	-0.00001	0.00041	-0.00102	-0.00061	3.14135
D24	-0.00672	-0.00002	0.00146	0.00155	0.00301	-0.00371
D25	-0.02425	0.00007	0.00397	0.00229	0.00626	-0.01799
D26	3.12495	0.00004	0.00365	0.00467	0.00832	3.13327
D27	3.11161	0.00010	0.00395	0.00231	0.00625	3.11786
D28	-0.02238	0.00006	0.00363	0.00468	0.00831	-0.01407
D29	-0.00249	0.00002	0.00047	0.00245	0.00292	0.00043
D30	3.13801	0.00001	0.00102	0.00117	0.00219	3.14020
D31	-3.13702	0.00001	-0.00058	-0.00011	-0.00069	-3.13771
D32	0.00348	0.00001	-0.00003	-0.00139	-0.00142	0.00207
D33	-0.01085	0.00007	0.00069	0.00310	0.00379	-0.00707
D34	3.12897	0.00006	0.00140	0.00163	0.00304	3.13200
D35	3.13676	0.00003	0.00098	0.00183	0.00281	3.13957
D36	-0.00661	0.00003	0.00169	0.00037	0.00206	-0.00455
D37	0.02483	-0.00007	-0.00443	-0.00140	-0.00583	0.01900
D38	-3.11193	-0.00009	-0.00555	-0.00144	-0.00699	-3.11892
D39	-3.12465	-0.00002	-0.00409	-0.00388	-0.00797	-3.13262
D40	0.02177	-0.00004	-0.00521	-0.00393	-0.00913	0.01264
D41	1.18482	0.00004	0.00016	-0.05799	-0.05783	1.12699
D42	-2.98866	-0.00014	-0.00169	-0.05827	-0.05997	-3.04862
D43	-0.89872	-0.00002	-0.00061	-0.05442	-0.05502	-0.95374
D44	-1.94898	0.00000	-0.00017	-0.05554	-0.05572	-2.00469
D45	0.16073	-0.00019	-0.00202	-0.05582	-0.05785	0.10288

```
   D46        2.25067  -0.00006  -0.00094  -0.05197  -0.05290
2.19776
   D47       -0.00755   0.00000   0.00214  -0.00127   0.00087  -
0.00669
   D48        3.13580   0.00001   0.00143   0.00017   0.00161
3.13740
   D49        3.12953   0.00001   0.00318  -0.00123   0.00195
3.13149
   D50       -0.01030   0.00002   0.00248   0.00022   0.00270  -
0.00761
   D51       -3.14056   0.00001  -0.00049   0.00170   0.00121  -
3.13935
   D52        0.00964   0.00000  -0.00216  -0.00055  -0.00271
0.00693
   D53        0.00574   0.00000  -0.00158   0.00165   0.00007
0.00581
   D54       -3.12725  -0.00002  -0.00325  -0.00060  -0.00385  -
3.13109
   D55        0.00501   0.00002  -0.00191   0.00129  -0.00062
0.00439
   D56       -3.13253  -0.00001  -0.00235   0.00017  -0.00218  -
3.13472
   D57       -3.13835   0.00001  -0.00120  -0.00017  -0.00137  -
3.13972
   D58        0.00729  -0.00002  -0.00164  -0.00129  -0.00293
0.00436
   D59        0.00079  -0.00001  -0.00023   0.00054   0.00031
0.00110
   D60        3.14006   0.00000   0.00017   0.00148   0.00165  -
3.14147
   D61       -3.13665  -0.00003  -0.00067  -0.00061  -0.00129  -
3.13793
   D62        0.00263  -0.00003  -0.00028   0.00033   0.00006
0.00268
   D63       -0.00563   0.00002   0.00119   0.00135   0.00254  -
0.00309
   D64        3.13405   0.00003   0.00192  -0.00004   0.00187
3.13593
   D65        3.13826   0.00002   0.00079   0.00042   0.00121
3.13947
   D66       -0.00524   0.00002   0.00152  -0.00098   0.00054  -
0.00469
   D67        0.00218  -0.00002  -0.00023  -0.00248  -0.00272  -
0.00054
   D68        3.13528   0.00000   0.00141  -0.00025   0.00115
3.13643
   D69       -3.13751  -0.00002  -0.00096  -0.00109  -0.00205  -
3.13955
   D70       -0.00440  -0.00001   0.00068   0.00114   0.00182  -
0.00258
         Item               Value     Threshold  Converged?
 Maximum Force            0.001553     0.000450     NO
```

```
 RMS     Force            0.000285     0.000300     YES
 Maximum Displacement     0.133477     0.001800     NO
 RMS     Displacement     0.017054     0.001200     NO
 Predicted change in Energy=-2.639981D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.792789   -5.417849    0.019721
      2          6           0       -3.422287   -5.391616    0.003178
      3          6           0       -2.705552   -4.153024   -0.012598
      4          6           0       -3.438453   -2.908309   -0.016702
      5          6           0       -4.870125   -2.986669    0.005358
      6          6           0       -5.523718   -4.195016    0.022664
      7          6           0       -1.307014   -4.124257   -0.021478
      8          6           0       -2.746380   -1.670619   -0.035055
      9          6           0       -1.328157   -1.660372   -0.027214
     10          6           0       -0.603155   -2.916509   -0.024481
     11          6           0        0.829048   -2.906563   -0.021780
     12          1           0        1.345725   -3.863917   -0.021562
     13          6           0        1.532402   -1.731811   -0.016620
     14          6           0        0.831006   -0.491455   -0.012495
     15          6           0       -0.541180   -0.458409   -0.017267
     16          1           0       -0.754472   -5.062007   -0.021364
     17          1           0       -5.326649   -6.364545    0.031964
     18          1           0       -2.848765   -6.316057    0.003649
     19          1           0       -5.454829   -2.073056    0.011811
     20          1           0       -6.610251   -4.221397    0.040511
     21          1           0        2.619278   -1.737286   -0.014730
     22          1           0        1.391320    0.439927   -0.003041
     23          1           0       -1.032667    0.507296   -0.008938
     24          6           0       -3.557020   -0.393751   -0.049752
     25          1           0       -4.140757   -0.276972    0.873711
     26          1           0       -2.945291    0.501490   -0.156320
     27          1           0       -4.270696   -0.389261   -0.882651
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                      1          2          3          4          5
    1  C    0.000000
    2  C    1.370853   0.000000
    3  C    2.440776   1.431107   0.000000
    4  C    2.851901   2.483438   1.444464   0.000000
    5  C    2.432452   2.807136   2.458879   1.433985   0.000000
    6  C    1.424635   2.418314   2.818699   2.450611   1.373895
    7  C    3.718294   2.466006   1.398862   2.453892   3.740400
    8  C    4.269955   3.782080   2.482842   1.418160   2.498782
    9  C    5.111214   4.278841   2.847936   2.451695   3.782282
```

This journal is © The Royal Society of Chemistry 2014

10	C	4.879723	3.751589	2.439095	2.835321	4.267652
11	C	6.157380	4.924424	3.747952	4.267504	5.699801
12	H	6.332280	5.006837	4.061590	4.878686	6.277507
13	C	7.320946	6.159830	4.880835	5.108185	6.524378
14	C	7.476461	6.488630	5.090612	4.906067	6.223288
15	C	6.532503	5.712943	4.281904	3.794233	5.013220
16	H	4.054173	2.688211	2.152450	3.441248	4.609376
17	H	1.086918	2.138695	3.429718	3.938682	3.408691
18	H	2.141557	1.087897	2.167830	3.458453	3.894962
19	H	3.409692	3.891547	3.447519	2.182712	1.084716
20	H	2.176027	3.396162	3.905658	3.433332	2.133970
21	H	8.275655	7.060803	5.847188	6.169879	7.592926
22	H	8.518055	7.561596	6.154644	5.876868	7.137739
23	H	7.017598	6.364557	4.951478	4.177826	5.189805
24	C	5.174312	4.999960	3.854673	2.517569	2.906975
25	H	5.251958	5.237710	4.227190	2.865310	2.937426
26	H	6.203452	5.914529	4.662899	3.448106	3.987277
27	H	5.135519	5.150538	4.168043	2.790717	2.809698

		6	7	8	9	10
6	C	0.000000				
7	C	4.217529	0.000000			
8	C	3.753600	2.844697	0.000000		
9	C	4.902003	2.463982	1.418282	0.000000	
10	C	5.084166	1.397885	2.479066	1.450350	0.000000
11	C	6.482262	2.458768	3.783044	2.491296	1.432240
12	H	6.877560	2.665484	4.642851	3.464866	2.166963
13	C	7.473805	3.712965	4.279260	2.861471	2.442166
14	C	7.355279	4.215266	3.766780	2.455315	2.817419
15	C	6.228122	3.744992	2.516481	1.436714	2.458891
16	H	4.847610	1.088428	3.933115	3.449676	2.150829
17	H	2.178481	4.602088	5.356792	6.174195	5.848379
18	H	3.413877	2.679854	4.646728	4.897816	4.074370
19	H	2.123105	4.627408	2.738585	4.147439	4.924578
20	H	1.086999	5.304488	4.630515	5.870600	6.147532
21	H	8.505893	4.594936	5.366111	3.948204	3.431433
22	H	8.324728	5.302181	4.644996	3.436189	3.904363
23	H	6.502482	4.639688	2.771427	2.187792	3.450675
24	C	4.280509	4.356604	1.512529	2.563720	3.884618
25	H	4.241218	4.861385	2.170805	3.261315	4.504279
26	H	5.360736	4.909141	2.184566	2.702857	4.145563
27	H	4.107728	4.845124	2.164218	3.317534	4.535890

		11	12	13	14	15
11	C	0.000000				
12	H	1.087880	0.000000			
13	C	1.369225	2.140269	0.000000		
14	C	2.415127	3.411528	1.424941	0.000000	
15	C	2.805531	3.893317	2.433371	1.372593	0.000000
16	H	2.674597	2.417901	4.039805	4.837744	4.608538
17	H	7.060675	7.125769	8.277148	8.509517	7.601683
18	H	5.015138	4.858742	6.341164	6.889628	6.295826
19	H	6.339004	7.032485	6.995617	6.481804	5.172222
20	H	7.554855	7.964245	8.514934	8.323916	7.141221

21	H	2.138266	2.478819	1.086891	2.179453	3.409403
22	H	3.393449	4.304126	2.176358	1.086974	2.131142
23	H	3.888519	4.976386	3.404885	2.114426	1.083612
24	C	5.054957	6.006643	5.262482	4.389272	3.016707
25	H	5.693471	6.615828	5.924017	5.054680	3.712642
26	H	5.087097	6.122725	5.005685	3.907307	2.592391
27	H	5.751982	6.660248	6.019004	5.176387	3.829225

		16	17	18	19	20
16	H	0.000000				
17	H	4.754393	0.000000			
18	H	2.441174	2.478520	0.000000		
19	H	5.570304	4.293450	4.979428	0.000000	
20	H	5.916130	2.498157	4.305547	2.439506	0.000000
21	H	4.736665	9.195187	7.131968	8.081129	9.558141
22	H	5.905593	9.562069	7.976321	7.292809	9.260398
23	H	5.576260	8.103219	7.060915	5.119977	7.312484
24	C	5.444969	6.228053	5.964745	2.534864	4.897064
25	H	5.929978	6.258868	6.236731	2.386541	4.727697
26	H	5.980835	7.269715	6.820107	3.599214	5.981332
27	H	5.911024	6.136414	6.159086	2.244415	4.583777

		21	22	23	24	25
21	H	0.000000				
22	H	2.499655	0.000000			
23	H	4.286594	2.424930	0.000000		
24	C	6.320836	5.018293	2.680654	0.000000	
25	H	6.972798	5.646814	3.324810	1.098713	0.000000
26	H	5.999716	4.339755	1.918302	1.089507	1.759575
27	H	7.074051	5.789619	3.471602	1.096848	1.764738

		26	27
26	H	0.000000	
27	H	1.754335	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.651180	-1.006833	0.010736
2	6	0	-2.451574	-1.670149	-0.003356
3	6	0	-1.211004	-0.956697	-0.009662
4	6	0	-1.222321	0.487719	-0.006660
5	6	0	-2.501000	1.136508	0.012499
6	6	0	-3.671777	0.417619	0.020641
7	6	0	0.014102	-1.631893	-0.016028
8	6	0	-0.003539	1.212749	-0.015590
9	6	0	1.229257	0.511584	-0.005327
10	6	0	1.228025	-0.938759	-0.009789

```
     11          6           0        2.472796   -1.647158   -0.004644
     12          1           0        2.440808   -2.734554   -0.009970
     13          6           0        3.669725   -0.982374    0.009537
     14          6           0        3.683460    0.442456    0.020791
     15          6           0        2.512174    1.158035    0.013962
     16          1           0        0.022976   -2.720273   -0.021267
     17          1           0       -4.587301   -1.559139    0.015763
     18          1           0       -2.417879   -2.757513   -0.008114
     19          1           0       -2.549829    2.220061    0.024090
     20          1           0       -4.625640    0.938638    0.036508
     21          1           0        4.607843   -1.531240    0.013194
     22          1           0        4.634711    0.968154    0.037401
     23          1           0        2.570107    2.240007    0.027932
     24          6           0       -0.066004    2.723969   -0.023095
     25          1           0       -0.517281    3.112715    0.900158
     26          1           0        0.912218    3.193217   -0.122660
     27          1           0       -0.677576    3.089268   -0.857129
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3941327      0.4478788
0.3397124
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9338900115 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860668923     A.U. after   11 cycles
             Convg  =    0.5391D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000221897    0.000169868   -0.000040252
      2        6           0.000241836    0.000279897   -0.000059219
      3        6           0.000370326   -0.000221255   -0.000015739
      4        6           0.000028662    0.000217376    0.000158983
      5        6          -0.000346307   -0.000475788   -0.000268655
      6        6           0.000167777    0.000142764    0.000080746
      7        6          -0.000181046    0.000368930    0.000026328
      8        6           0.000984268   -0.000793850    0.000717797
      9        6          -0.000482209    0.000097855   -0.000154884
     10        6          -0.000153775   -0.000312970    0.000019313
     11        6          -0.000451586   -0.000216239   -0.000023072
```

```
     12        1           0.000257711    0.000109861   -0.000035497
     13        6           0.000070904    0.000380156   -0.000088507
     14        6          -0.000180854   -0.000003356    0.000119397
     15        6           0.000013472   -0.000267941   -0.000177297
     16        1           0.000037472   -0.000046550    0.000028824
     17        1           0.000132170   -0.000084981    0.000028770
     18        1          -0.000210697   -0.000161346   -0.000011881
     19        1           0.000018103   -0.000220961   -0.000015445
     20        1          -0.000114231    0.000041353   -0.000003879
     21        1          -0.000001611   -0.000159239    0.000055282
     22        1           0.000035721    0.000114783   -0.000031838
     23        1          -0.000125714    0.000057895   -0.000026615
     24        6          -0.000506564    0.001237706   -0.000080745
     25        1           0.000253807   -0.000273448   -0.000125906
     26        1           0.000378365   -0.000002795   -0.000003587
     27        1          -0.000014103    0.000022275   -0.000072420
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.001237706 RMS     0.000285265


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.001136826 RMS     0.000223280
 Search for a local minimum.
 Step number  41 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   31   32   33   35
34
                                                     36   37   38   39
40
                                                     41
 DE= -1.48D-05 DEPred=-2.64D-05 R= 5.61D-01
 SS=  1.41D+00  RLast= 1.41D-01 DXNew= 2.3784D-01 4.2426D-01
 Trust test= 5.61D-01 RLast= 1.41D-01 DXMaxT set to 2.38D-01
     Eigenvalues ---    0.00006   0.00220   0.01102   0.01554
0.01639
     Eigenvalues ---    0.01774   0.01811   0.01825   0.01897
0.01939
     Eigenvalues ---    0.01971   0.01978   0.02009   0.02067
0.02098
     Eigenvalues ---    0.02107   0.02145   0.02165   0.02223
0.02227
     Eigenvalues ---    0.02332   0.02355   0.05368   0.06306
0.08251
     Eigenvalues ---    0.10432   0.13537   0.15465   0.15769
0.15966
     Eigenvalues ---    0.15999   0.16001   0.16002   0.16013
0.16059
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.16583   0.17399   0.21205   0.22006
0.22561
     Eigenvalues ---    0.22734   0.22970   0.24082   0.24615
0.24681
     Eigenvalues ---    0.25235   0.27639   0.31072   0.33017
0.33076
     Eigenvalues ---    0.33590   0.33630   0.33635   0.33682
0.33683
     Eigenvalues ---    0.33933   0.34242   0.34768   0.36256
0.37371
     Eigenvalues ---    0.37502   0.38045   0.38512   0.39535
0.40134
     Eigenvalues ---    0.40566   0.40923   0.43571   0.44476
0.46142
     Eigenvalues ---    0.49335   0.49814   0.50399   0.51191
0.55923
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   6.38D-05 Eigenvector:
                          D44       D46       D45       D41       D43
   1                    0.43350   0.42907   0.42734   0.37664
0.37220
                          D42       D38       D27       D37       D25
   1                    0.37047   0.06630  -0.05523   0.04660  -
0.04216
```

This journal is © The Royal Society of Chemistry 2014

```
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    41   40   39   38
37
 RFO step:  Lambda=-1.30739169D-05.
 DIIS coeffs:      0.81167      0.15488      0.91104     -0.10679
-0.77080
 Iteration  1 RMS(Cart)=  0.01901670 RMS(Int)=  0.00042403
 Iteration  2 RMS(Cart)=  0.00044220 RMS(Int)=  0.00001292
 Iteration  3 RMS(Cart)=  0.00000025 RMS(Int)=  0.00001291
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59054   0.00003   0.00047   0.00003   0.00050
2.59104
    R2        2.69217  -0.00017  -0.00060  -0.00015  -0.00074
2.69143
    R3        2.05398   0.00001  -0.00009   0.00027   0.00019
2.05416
    R4        2.70440  -0.00004  -0.00030  -0.00005  -0.00035
2.70405
    R5        2.05583   0.00003  -0.00001   0.00008   0.00007
2.05589
    R6        2.72964   0.00026   0.00063  -0.00040   0.00022
2.72986
    R7        2.64347  -0.00017  -0.00076  -0.00001  -0.00077
2.64270
    R8        2.70984   0.00036  -0.00018   0.00021   0.00003
2.70987
    R9        2.67993   0.00032  -0.00070   0.00020  -0.00051
2.67942
   R10        2.59628  -0.00029  -0.00017  -0.00031  -0.00048
2.59581
   R11        2.04982  -0.00020  -0.00024   0.00018  -0.00006
2.04975
   R12        2.05413   0.00011   0.00029   0.00020   0.00049
2.05462
   R13        2.64162  -0.00029  -0.00046  -0.00029  -0.00074
2.64088
   R14        2.05683   0.00006   0.00007   0.00016   0.00023
2.05706
   R15        2.68016  -0.00099   0.00031  -0.00159  -0.00129
2.67887
   R16        2.85827   0.00077   0.00102   0.00262   0.00363
2.86190
   R17        2.74076  -0.00019   0.00042   0.00006   0.00047
2.74123
   R18        2.71500  -0.00027  -0.00010  -0.00043  -0.00054
2.71446
   R19        2.70654  -0.00004  -0.00042   0.00015  -0.00028
2.70626
   R20        2.05580   0.00003  -0.00001   0.00007   0.00005
2.05585
```

This journal is © The Royal Society of Chemistry 2014

R21	2.58746	0.00027	0.00053	0.00009	0.00063
2.58809					
R22	2.69275	-0.00004	-0.00083	0.00011	-0.00071
2.69204					
R23	2.05393	0.00000	-0.00008	0.00024	0.00016
2.05409					
R24	2.59382	-0.00024	-0.00006	-0.00044	-0.00050
2.59333					
R25	2.05408	0.00012	0.00030	0.00019	0.00050
2.05458					
R26	2.04773	0.00011	-0.00050	0.00051	0.00001
2.04774					
R27	2.07627	-0.00027	0.00034	-0.00159	-0.00125
2.07502					
R28	2.05887	0.00021	0.00057	-0.00125	-0.00068
2.05819					
R29	2.07274	0.00006	0.00047	0.00079	0.00127
2.07401					
A1	2.09039	0.00006	-0.00027	0.00083	0.00056
2.09095					
A2	2.10348	-0.00019	0.00027	-0.00163	-0.00136
2.10212					
A3	2.08931	0.00013	0.00000	0.00080	0.00081
2.09012					
A4	2.11460	0.00011	0.00046	-0.00009	0.00035
2.11495					
A5	2.10689	-0.00032	-0.00052	-0.00175	-0.00226
2.10463					
A6	2.06170	0.00022	0.00007	0.00184	0.00191
2.06361					
A7	2.08485	-0.00010	-0.00019	-0.00079	-0.00100
2.08386					
A8	2.11598	0.00006	0.00021	0.00114	0.00138
2.11736					
A9	2.08235	0.00004	-0.00001	-0.00034	-0.00038
2.08197					
A10	2.04816	-0.00020	-0.00054	0.00095	0.00040
2.04856					
A11	2.09958	-0.00032	0.00018	-0.00014	-0.00001
2.09957					
A12	2.13543	0.00052	0.00039	-0.00081	-0.00038
2.13506					
A13	2.12141	0.00020	0.00076	-0.00020	0.00054
2.12195					
A14	2.08545	0.00001	0.00010	-0.00050	-0.00040
2.08505					
A15	2.07632	-0.00020	-0.00084	0.00071	-0.00013
2.07618					
A16	2.10693	-0.00006	-0.00016	-0.00068	-0.00083
2.10610					
A17	2.08523	0.00008	-0.00011	0.00063	0.00052
2.08576					

This journal is © The Royal Society of Chemistry 2014

A18	2.09102	-0.00001	0.00027	0.00005	0.00031
2.09133					
A19	2.11903	-0.00001	0.00024	-0.00001	0.00020
2.11923					
A20	2.08267	0.00001	-0.00015	0.00015	0.00001
2.08268					
A21	2.08147	-0.00001	-0.00008	-0.00014	-0.00020
2.08127					
A22	2.08774	0.00007	-0.00006	0.00081	0.00067
2.08841					
A23	2.06615	0.00107	-0.00015	-0.00220	-0.00232
2.06383					
A24	2.12926	-0.00114	0.00023	0.00144	0.00169
2.13095					
A25	2.08704	0.00028	0.00002	-0.00064	-0.00067
2.08637					
A26	2.15774	-0.00056	0.00074	-0.00010	0.00069
2.15843					
A27	2.03840	0.00029	-0.00076	0.00074	-0.00001
2.03839					
A28	2.09047	-0.00006	-0.00004	0.00041	0.00035
2.09081					
A29	2.10540	0.00032	0.00004	0.00035	0.00042
2.10582					
A30	2.08732	-0.00027	0.00000	-0.00076	-0.00076
2.08655					
A31	2.05875	0.00028	0.00021	0.00175	0.00196
2.06071					
A32	2.11723	0.00001	0.00042	-0.00003	0.00038
2.11760					
A33	2.10721	-0.00029	-0.00063	-0.00171	-0.00234
2.10487					
A34	2.08747	0.00006	-0.00030	0.00051	0.00021
2.08768					
A35	2.10524	-0.00019	0.00026	-0.00148	-0.00123
2.10402					
A36	2.09048	0.00013	0.00004	0.00097	0.00101
2.09149					
A37	2.10951	-0.00017	-0.00019	-0.00053	-0.00072
2.10879					
A38	2.08536	0.00012	-0.00022	0.00067	0.00045
2.08581					
A39	2.08832	0.00006	0.00041	-0.00014	0.00027
2.08859					
A40	2.12643	0.00009	0.00085	0.00009	0.00093
2.12736					
A41	2.09115	-0.00013	0.00040	0.00005	0.00045
2.09160					
A42	2.06560	0.00005	-0.00125	-0.00013	-0.00137
2.06423					
A43	1.94583	-0.00034	-0.00165	-0.00285	-0.00450
1.94134					

```
   A44        1.97545  -0.00040   0.00128  -0.00039   0.00089
1.97634
   A45        1.93859   0.00018   0.00133  -0.00221  -0.00088
1.93770
   A46        1.86835   0.00030   0.00054   0.00128   0.00182
1.87017
   A47        1.86723   0.00016   0.00003   0.00149   0.00151
1.86874
   A48        1.86261   0.00015  -0.00161   0.00313   0.00151
1.86412
    D1       -0.00106   0.00003   0.00086  -0.00035   0.00051  -
0.00055
    D2        3.13844   0.00003   0.00200   0.00044   0.00243
3.14088
    D3       -3.14122   0.00002   0.00013  -0.00022  -0.00009  -
3.14131
    D4       -0.00171   0.00002   0.00127   0.00057   0.00184
0.00013
    D5        0.00316   0.00000  -0.00148  -0.00064  -0.00212
0.00104
    D6       -3.13662  -0.00002  -0.00316  -0.00137  -0.00453  -
3.14116
    D7       -3.13986   0.00001  -0.00075  -0.00078  -0.00153  -
3.14139
    D8        0.00355  -0.00002  -0.00244  -0.00151  -0.00394  -
0.00040
    D9       -0.00447   0.00000   0.00185   0.00177   0.00362  -
0.00085
   D10        3.13489   0.00003   0.00349   0.00241   0.00591
3.14080
   D11        3.13915   0.00000   0.00074   0.00101   0.00174
3.14090
   D12       -0.00466   0.00003   0.00238   0.00165   0.00403  -
0.00064
   D13        0.00773  -0.00005  -0.00385  -0.00214  -0.00599
0.00174
   D14       -3.13932   0.00003   0.00012  -0.00163  -0.00150  -
3.14082
   D15       -3.13168  -0.00008  -0.00547  -0.00277  -0.00823  -
3.13991
   D16        0.00445   0.00000  -0.00149  -0.00226  -0.00374
0.00071
   D17       -3.13119  -0.00010  -0.00621  -0.00137  -0.00758  -
3.13877
   D18        0.00536  -0.00004  -0.00452  -0.00124  -0.00576  -
0.00040
   D19        0.00818  -0.00007  -0.00457  -0.00073  -0.00530
0.00288
   D20       -3.13846  -0.00001  -0.00288  -0.00060  -0.00348
3.14125
   D21       -0.00582   0.00008   0.00333   0.00120   0.00452  -
0.00130
```

This journal is © The Royal Society of Chemistry 2014

D22	3.13230	0.00004	0.00403	0.00253	0.00656	3.13886
D23	3.14135	0.00000	-0.00075	0.00067	-0.00007	3.14129
D24	-0.00371	-0.00003	-0.00004	0.00201	0.00197	-0.00174
D25	-0.01799	0.00009	0.00777	0.00517	0.01294	-0.00505
D26	3.13327	-0.00003	0.00532	0.00015	0.00548	3.13875
D27	3.11786	0.00017	0.01195	0.00571	0.01766	3.13552
D28	-0.01407	0.00005	0.00949	0.00069	0.01020	-0.00386
D29	0.00043	-0.00005	-0.00070	0.00019	-0.00051	-0.00008
D30	3.14020	-0.00003	0.00099	0.00092	0.00191	-3.14107
D31	-3.13771	-0.00002	-0.00141	-0.00114	-0.00254	-3.14025
D32	0.00207	0.00000	0.00029	-0.00041	-0.00012	0.00195
D33	-0.00707	0.00005	0.00425	0.00074	0.00499	-0.00208
D34	3.13200	0.00008	0.00533	0.00162	0.00695	3.13896
D35	3.13957	-0.00001	0.00256	0.00062	0.00317	-3.14045
D36	-0.00455	0.00002	0.00364	0.00149	0.00513	0.00058
D37	0.01900	-0.00010	-0.00806	-0.00512	-0.01318	0.00583
D38	-3.11892	-0.00013	-0.00910	-0.00566	-0.01476	-3.13369
D39	-3.13262	0.00004	-0.00554	0.00007	-0.00545	-3.13807
D40	0.01264	0.00001	-0.00658	-0.00047	-0.00703	0.00561
D41	1.12699	0.00012	-0.01491	-0.03936	-0.05426	1.07273
D42	-3.04862	-0.00002	-0.01448	-0.04006	-0.05455	-3.10317
D43	-0.95374	0.00003	-0.01474	-0.03788	-0.05262	-1.00636
D44	-2.00469	-0.00001	-0.01741	-0.04450	-0.06190	-2.06659
D45	0.10288	-0.00015	-0.01698	-0.04520	-0.06219	0.04069
D46	2.19776	-0.00010	-0.01724	-0.04302	-0.06026	2.13750
D47	-0.00669	0.00003	0.00214	0.00220	0.00435	-0.00233

```
   D48        3.13740   0.00000   0.00107   0.00134   0.00241
3.13982
   D49        3.13149   0.00006   0.00312   0.00271   0.00583
3.13732
   D50       -0.00761   0.00003   0.00205   0.00184   0.00389  -
0.00372
   D51       -3.13935  -0.00002  -0.00077  -0.00042  -0.00119  -
3.14054
   D52        0.00693   0.00000  -0.00059  -0.00231  -0.00290
0.00403
   D53        0.00581  -0.00005  -0.00178  -0.00094  -0.00273
0.00308
   D54       -3.13109  -0.00003  -0.00160  -0.00283  -0.00444  -
3.13553
   D55        0.00439  -0.00002  -0.00138  -0.00140  -0.00278
0.00161
   D56       -3.13472  -0.00002  -0.00202  -0.00257  -0.00459  -
3.13931
   D57       -3.13972   0.00002  -0.00030  -0.00053  -0.00082  -
3.14055
   D58        0.00436   0.00001  -0.00093  -0.00170  -0.00264
0.00172
   D59        0.00110  -0.00002  -0.00054   0.00054   0.00000
0.00110
   D60       -3.14147  -0.00003  -0.00081   0.00034  -0.00048
3.14124
   D61       -3.13793  -0.00003  -0.00120  -0.00066  -0.00187  -
3.13980
   D62        0.00268  -0.00004  -0.00147  -0.00087  -0.00234
0.00034
   D63       -0.00309  -0.00001   0.00085   0.00041   0.00126  -
0.00183
   D64        3.13593   0.00003   0.00248   0.00136   0.00384
3.13977
   D65        3.13947   0.00000   0.00112   0.00062   0.00174
3.14121
   D66       -0.00469   0.00003   0.00275   0.00156   0.00432  -
0.00038
   D67       -0.00054   0.00005   0.00036  -0.00018   0.00018  -
0.00036
   D68        3.13643   0.00002   0.00020   0.00168   0.00187
3.13831
   D69       -3.13955   0.00001  -0.00127  -0.00113  -0.00240
3.14123
   D70       -0.00258  -0.00001  -0.00144   0.00073  -0.00071  -
0.00329
         Item               Value     Threshold  Converged?
 Maximum Force            0.001137     0.000450     NO
 RMS     Force            0.000223     0.000300     YES
 Maximum Displacement     0.140716     0.001800     NO
 RMS     Displacement     0.019013     0.001200     NO
 Predicted change in Energy=-1.730719D-05
```

This journal is © The Royal Society of Chemistry 2014

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.793560	-5.416084	0.016597
2	6	0	-3.422687	-5.390940	0.009751
3	6	0	-2.704537	-4.153344	-0.002869
4	6	0	-3.437256	-2.908397	-0.009567
5	6	0	-4.869128	-2.986008	-0.000843
6	6	0	-5.524009	-4.193427	0.011812
7	6	0	-1.306395	-4.124324	-0.008928
8	6	0	-2.745006	-1.671055	-0.023021
9	6	0	-1.327450	-1.660351	-0.023666
10	6	0	-0.602748	-2.916937	-0.017891
11	6	0	0.829301	-2.906401	-0.020753
12	1	0	1.348271	-3.862540	-0.017300
13	6	0	1.532782	-1.731341	-0.026841
14	6	0	0.831794	-0.491182	-0.029056
15	6	0	-0.540155	-0.458902	-0.027319
16	1	0	-0.753593	-5.062043	-0.003560
17	1	0	-5.326999	-6.363158	0.026445
18	1	0	-2.851998	-6.317164	0.013961
19	1	0	-5.453021	-2.071897	-0.002925
20	1	0	-6.610951	-4.219010	0.017693
21	1	0	2.619737	-1.738111	-0.028624
22	1	0	1.392004	0.440610	-0.032165
23	1	0	-1.030822	0.507263	-0.025981
24	6	0	-3.559327	-0.394207	-0.033379
25	1	0	-4.183322	-0.313246	0.866506
26	1	0	-2.947269	0.505390	-0.081857
27	1	0	-4.235084	-0.365210	-0.897703

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.371120	0.000000			
3	C	2.441087	1.430923	0.000000		
4	C	2.851094	2.482660	1.444582	0.000000	
5	C	2.431313	2.806421	2.459295	1.434000	0.000000
6	C	1.424243	2.418593	2.819795	2.450775	1.373641
7	C	3.718820	2.466447	1.398457	2.453375	3.740173
8	C	4.268885	3.781252	2.482701	1.417888	2.498297
9	C	5.110878	4.278835	2.848125	2.451347	3.781715
10	C	4.879532	3.751468	2.438533	2.834533	4.266973
11	C	6.157635	4.924760	3.747425	4.266572	5.699019
12	H	6.335356	5.009868	4.063253	4.879725	6.278903
13	C	7.321327	6.160413	4.880732	5.107547	6.523750

14	C	7.476720	6.489202	5.090948	4.905924	6.222978
15	C	6.532001	5.712737	4.281828	3.793881	5.012681
16	H	4.055500	2.689315	2.152188	3.440970	4.609507
17	H	1.087016	2.138198	3.429496	3.937994	3.408157
18	H	2.140471	1.087932	2.168904	3.458724	3.894308
19	H	3.408644	3.890818	3.447693	2.182449	1.084682
20	H	2.176211	3.396837	3.907020	3.433772	2.134147
21	H	8.275657	7.060845	5.846530	6.169044	7.592175
22	H	8.518477	7.562406	6.155236	5.876914	7.137540
23	H	7.017553	6.364833	4.952082	4.178269	5.190007
24	C	5.171564	4.998786	3.855218	2.517264	2.904147
25	H	5.209000	5.205340	4.205826	2.838825	2.892452
26	H	6.203413	5.916174	4.665722	3.449530	3.986222
27	H	5.163252	5.171211	4.182495	2.809469	2.841646

		6	7	8	9	10
6	C	0.000000				
7	C	4.218232	0.000000			
8	C	3.753189	2.843999	0.000000		
9	C	4.901922	2.464107	1.417597	0.000000	
10	C	5.084203	1.397491	2.478208	1.450598	0.000000
11	C	6.482441	2.458591	3.781766	2.490828	1.432091
12	H	6.880303	2.667555	4.643012	3.465423	2.168096
13	C	7.474066	3.713168	4.278215	2.861115	2.442582
14	C	7.355577	4.215682	3.766382	2.455467	2.818212
15	C	6.227922	3.744700	2.516089	1.436428	2.458849
16	H	4.848876	1.088547	3.932544	3.449816	2.150452
17	H	2.178706	4.602053	5.355835	6.173759	5.847816
18	H	3.413196	2.682902	4.647488	4.900161	4.076970
19	H	2.122769	4.626770	2.737594	4.146099	4.923358
20	H	1.087259	5.305468	4.630255	5.870590	6.147777
21	H	8.505928	4.594443	5.365166	3.947956	3.431349
22	H	8.325111	5.302878	4.644790	3.436501	3.905427
23	H	6.502819	4.639809	2.771914	2.187817	3.450863
24	C	4.277393	4.357760	1.514452	2.566026	3.886613
25	H	4.193298	4.854627	2.168791	3.280717	4.514628
26	H	5.359781	4.912437	2.186615	2.705112	4.148878
27	H	4.140506	4.847482	2.165787	3.300859	4.525400

		11	12	13	14	15
11	C	0.000000				
12	H	1.087908	0.000000			
13	C	1.369558	2.139193	0.000000		
14	C	2.415234	3.410709	1.424564	0.000000	
15	C	2.804586	3.892429	2.432317	1.372329	0.000000
16	H	2.674442	2.420089	4.040004	4.838065	4.608148
17	H	7.060554	7.128411	8.277269	8.509636	7.601119
18	H	5.018612	4.865020	6.344899	6.893057	6.298060
19	H	6.337529	7.033077	6.994140	6.480604	5.170938
20	H	7.555247	7.967277	8.515332	8.324262	7.141079
21	H	2.137902	2.475874	1.086978	2.179811	3.409002
22	H	3.394002	4.303398	2.176515	1.087236	2.131287
23	H	3.887568	4.975473	3.403442	2.113348	1.083620
24	C	5.056810	6.009501	5.264745	4.392193	3.019871

This journal is © The Royal Society of Chemistry 2014

25	H	5.712973	6.631524	5.956753	5.097556	3.754038
26	H	5.089845	6.126552	5.007679	3.908613	2.593652
27	H	5.733645	6.646825	5.991077	5.142341	3.797216

		16	17	18	19	20
16	H	0.000000				
17	H	4.754981	0.000000			
18	H	2.445186	2.475460	0.000000		
19	H	5.570062	4.293212	4.978745	0.000000	
20	H	5.917752	2.499195	4.304880	2.439534	0.000000
21	H	4.735875	9.194820	7.135084	8.079697	9.558379
22	H	5.906234	9.562411	7.980050	7.291633	9.260769
23	H	5.576247	8.103245	7.063363	5.119418	7.312825
24	C	5.446258	6.225481	5.965231	2.530147	4.893275
25	H	5.922088	6.214107	6.208566	2.336856	4.676415
26	H	5.984535	7.269924	6.823892	3.595474	5.979334
27	H	5.914433	6.166175	6.178173	2.279644	4.618925

		21	22	23	24	25
21	H	0.000000				
22	H	2.500833	0.000000			
23	H	4.285825	2.423751	0.000000		
24	C	6.323522	5.021215	2.684407	0.000000	
25	H	7.008075	5.697383	3.377577	1.098052	0.000000
26	H	6.002307	4.340041	1.917262	1.089147	1.759939
27	H	7.044767	5.750011	3.433425	1.097518	1.765733

		26	27
26	H	0.000000	
27	H	1.755568	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.650826	-1.006428	0.003186
2	6	0	-2.451214	-1.670423	-0.000206
3	6	0	-1.210224	-0.958045	-0.002105
4	6	0	-1.221852	0.486489	-0.001493
5	6	0	-2.500539	1.135562	0.003250
6	6	0	-3.671650	0.417661	0.005555
7	6	0	0.014935	-1.632331	-0.004618
8	6	0	-0.003411	1.211609	-0.004290
9	6	0	1.229364	0.511725	-0.001475
10	6	0	1.228233	-0.938871	-0.003114
11	6	0	2.473486	-1.646140	-0.002483
12	1	0	2.444528	-2.733660	-0.004749
13	6	0	3.670455	-0.980604	0.001658
14	6	0	3.683880	0.443887	0.006795

```
     15          6           0        2.512091    1.158168    0.005493
     16          1           0        0.024473   -2.720836   -0.004754
     17          1           0       -4.586535   -1.559646    0.004870
     18          1           0       -2.420430   -2.757919   -0.001374
     19          1           0       -2.548826    2.219164    0.006426
     20          1           0       -4.625630    0.939240    0.008656
     21          1           0        4.608238   -1.530224    0.002420
     22          1           0        4.635086    0.970447    0.011804
     23          1           0        2.570545    2.240187    0.012691
     24          6           0       -0.069716    2.724606   -0.007300
     25          1           0       -0.574649    3.102275    0.891659
     26          1           0        0.910536    3.197584   -0.047770
     27          1           0       -0.635396    3.092187   -0.873000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3944924      0.4478698
0.3397126
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9621583687 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860680491     A.U. after   11 cycles
             Convg  =    0.5091D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000047393   -0.000152946    0.000042782
      2        6          -0.000036548    0.000018705   -0.000020781
      3        6          -0.000120784   -0.000053137   -0.000047230
      4        6          -0.000004393   -0.000037275    0.000002936
      5        6          -0.000279252   -0.000152085   -0.000006335
      6        6          -0.000075461    0.000078548   -0.000050756
      7        6           0.000079402   -0.000063180    0.000136230
      8        6           0.000116612    0.000149427    0.000178184
      9        6          -0.000202854   -0.000117980    0.000063130
     10        6           0.000042090    0.000021580   -0.000051108
     11        6          -0.000010728    0.000034556   -0.000009551
     12        1           0.000039713    0.000008648   -0.000006434
     13        6           0.000121240   -0.000093317    0.000032149
     14        6           0.000034568    0.000135689   -0.000047471
     15        6          -0.000154513    0.000170745    0.000001759
```

```
     16        1          -0.000000950    0.000009714   -0.000064511
     17        1           0.000082691    0.000010340   -0.000013619
     18        1          -0.000028292   -0.000030147    0.000001714
     19        1          -0.000001777   -0.000220359   -0.000008850
     20        1           0.000069534    0.000041384    0.000042300
     21        1          -0.000057058   -0.000066021   -0.000010968
     22        1          -0.000067212   -0.000042167    0.000042964
     23        1          -0.000248386    0.000016482   -0.000072082
     24        6           0.000030115    0.000045802   -0.000350661
     25        1           0.000199563    0.000086362   -0.000116597
     26        1           0.000434933    0.000150891    0.000198926
     27        1          -0.000009643    0.000049744    0.000133881
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000434933 RMS     0.000113369


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.001431817 RMS     0.000226179
 Search for a local minimum.
 Step number  42 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   35   34   36   37
38
                                                     39   40   41   42
 DE= -1.16D-05 DEPred=-1.73D-05 R= 6.68D-01
 SS=  1.41D+00  RLast= 1.48D-01 DXNew= 4.0000D-01 4.4458D-01
 Trust test= 6.68D-01 RLast= 1.48D-01 DXMaxT set to 4.00D-01
     Eigenvalues ---    0.00044   0.00113   0.01134   0.01547
0.01678
     Eigenvalues ---    0.01763   0.01808   0.01825   0.01906
0.01934
     Eigenvalues ---    0.01973   0.01977   0.02043   0.02065
0.02098
     Eigenvalues ---    0.02107   0.02145   0.02165   0.02223
0.02226
     Eigenvalues ---    0.02333   0.02354   0.05164   0.06333
0.08199
     Eigenvalues ---    0.10284   0.14145   0.15113   0.15686
0.15924
     Eigenvalues ---    0.15994   0.16000   0.16002   0.16006
0.16014
     Eigenvalues ---    0.16689   0.17262   0.21021   0.22006
0.22539
     Eigenvalues ---    0.22621   0.22948   0.24154   0.24587
0.24665
     Eigenvalues ---    0.25237   0.27866   0.31052   0.32894
0.33261
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.33590   0.33623   0.33632   0.33680
0.33682
     Eigenvalues ---    0.33900   0.34222   0.34741   0.35579
0.37455
     Eigenvalues ---    0.37575   0.38274   0.38447   0.39577
0.40302
     Eigenvalues ---    0.40441   0.40995   0.43401   0.44891
0.45635
     Eigenvalues ---    0.48589   0.49320   0.49859   0.51232
0.57125
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    42   41   40   39
38
 RFO step:  Lambda=-1.31751320D-05.
 DIIS coeffs:      1.00694     -0.06097     -0.60643     -1.72159
2.38205
 Iteration  1 RMS(Cart)=  0.03531757 RMS(Int)=  0.00193842
 Iteration  2 RMS(Cart)=  0.00201616 RMS(Int)=  0.00001476
 Iteration  3 RMS(Cart)=  0.00000526 RMS(Int)=  0.00001418
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00001418
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
```

This journal is © The Royal Society of Chemistry 2014

R1	2.59104	-0.00015	-0.00066	0.00027	-0.00039
2.59065					
R2	2.69143	0.00007	0.00041	-0.00021	0.00019
2.69162					
R3	2.05416	-0.00005	0.00020	-0.00044	-0.00024
2.05393					
R4	2.70405	0.00001	0.00035	-0.00019	0.00016
2.70422					
R5	2.05589	0.00001	0.00024	-0.00024	-0.00001
2.05589					
R6	2.72986	0.00028	0.00078	0.00095	0.00173
2.73160					
R7	2.64270	0.00019	0.00034	-0.00020	0.00012
2.64282					
R8	2.70987	0.00033	0.00088	0.00005	0.00093
2.71080					
R9	2.67942	0.00062	0.00042	0.00022	0.00065
2.68007					
R10	2.59581	-0.00001	-0.00044	0.00028	-0.00016
2.59564					
R11	2.04975	-0.00018	0.00005	-0.00058	-0.00054
2.04921					
R12	2.05462	-0.00007	0.00010	-0.00038	-0.00027
2.05435					
R13	2.64088	0.00000	0.00031	-0.00014	0.00017
2.64104					
R14	2.05706	-0.00001	0.00019	-0.00027	-0.00007
2.05698					
R15	2.67887	-0.00062	-0.00121	0.00111	-0.00009
2.67878					
R16	2.86190	-0.00007	-0.00033	-0.00001	-0.00034
2.86156					
R17	2.74123	-0.00019	-0.00202	0.00067	-0.00134
2.73989					
R18	2.71446	-0.00015	-0.00064	0.00046	-0.00017
2.71428					
R19	2.70626	0.00002	-0.00001	-0.00029	-0.00030
2.70596					
R20	2.05585	0.00001	0.00024	-0.00024	0.00001
2.05586					
R21	2.58809	0.00005	0.00012	0.00027	0.00039
2.58848					
R22	2.69204	0.00023	0.00060	-0.00038	0.00021
2.69225					
R23	2.05409	-0.00006	0.00019	-0.00043	-0.00024
2.05385					
R24	2.59333	0.00004	0.00009	0.00041	0.00050
2.59382					
R25	2.05458	-0.00007	0.00011	-0.00037	-0.00026
2.05432					
R26	2.04774	0.00013	0.00094	-0.00088	0.00006
2.04780					

This journal is © The Royal Society of Chemistry 2014

R27	2.07502	-0.00020	0.00014	0.00061	0.00075
2.07577					
R28	2.05819	0.00036	0.00114	0.00080	0.00194
2.06013					
R29	2.07401	-0.00010	-0.00256	0.00006	-0.00250
2.07151					
A1	2.09095	-0.00004	-0.00045	-0.00023	-0.00068
2.09027					
A2	2.10212	-0.00005	-0.00011	-0.00017	-0.00028
2.10184					
A3	2.09012	0.00009	0.00055	0.00040	0.00095
2.09107					
A4	2.11495	0.00007	0.00026	0.00029	0.00056
2.11551					
A5	2.10463	-0.00007	-0.00009	-0.00029	-0.00038
2.10425					
A6	2.06361	0.00001	-0.00018	0.00000	-0.00018
2.06343					
A7	2.08386	0.00012	0.00051	0.00005	0.00057
2.08443					
A8	2.11736	-0.00022	-0.00159	-0.00031	-0.00193
2.11543					
A9	2.08197	0.00010	0.00108	0.00026	0.00136
2.08333					
A10	2.04856	-0.00028	-0.00126	-0.00053	-0.00179
2.04677					
A11	2.09957	-0.00035	-0.00185	-0.00013	-0.00193
2.09764					
A12	2.13506	0.00063	0.00308	0.00066	0.00371
2.13877					
A13	2.12195	0.00007	0.00053	0.00035	0.00090
2.12285					
A14	2.08505	0.00009	0.00089	-0.00012	0.00076
2.08582					
A15	2.07618	-0.00016	-0.00145	-0.00022	-0.00168
2.07451					
A16	2.10610	0.00006	0.00034	0.00008	0.00042
2.10652					
A17	2.08576	0.00001	0.00037	0.00014	0.00051
2.08627					
A18	2.09133	-0.00007	-0.00071	-0.00022	-0.00093
2.09040					
A19	2.11923	-0.00001	-0.00030	0.00021	-0.00006
2.11917					
A20	2.08268	0.00001	0.00006	-0.00020	-0.00016
2.08252					
A21	2.08127	0.00000	0.00022	0.00000	0.00021
2.08148					
A22	2.08841	0.00001	-0.00010	-0.00037	-0.00039
2.08802					
A23	2.06383	0.00143	0.00916	0.00119	0.01031
2.07414					

```
   A24        2.13095  -0.00143  -0.00908  -0.00083  -0.00994
2.12101
   A25        2.08637   0.00039   0.00198   0.00025   0.00228
2.08865
   A26        2.15843  -0.00067  -0.00371   0.00022  -0.00353
2.15490
   A27        2.03839   0.00028   0.00172  -0.00047   0.00124
2.03963
   A28        2.09081  -0.00013  -0.00120  -0.00021  -0.00138
2.08943
   A29        2.10582   0.00024   0.00165   0.00014   0.00175
2.10757
   A30        2.08655  -0.00010  -0.00045   0.00007  -0.00037
2.08618
   A31        2.06071   0.00005   0.00047   0.00016   0.00062
2.06133
   A32        2.11760  -0.00002  -0.00042   0.00024  -0.00017
2.11743
   A33        2.10487  -0.00003  -0.00005  -0.00040  -0.00046
2.10442
   A34        2.08768   0.00003   0.00041  -0.00003   0.00038
2.08806
   A35        2.10402  -0.00008  -0.00059  -0.00028  -0.00088
2.10314
   A36        2.09149   0.00005   0.00018   0.00031   0.00050
2.09199
   A37        2.10879  -0.00007  -0.00036  -0.00006  -0.00042
2.10837
   A38        2.08581   0.00007   0.00049  -0.00001   0.00048
2.08629
   A39        2.08859   0.00000  -0.00013   0.00007  -0.00006
2.08853
   A40        2.12736  -0.00012  -0.00095   0.00025  -0.00069
2.12667
   A41        2.09160  -0.00016  -0.00109  -0.00018  -0.00127
2.09032
   A42        2.06423   0.00028   0.00201  -0.00007   0.00195
2.06617
   A43        1.94134   0.00007   0.00276   0.00071   0.00347
1.94481
   A44        1.97634  -0.00046  -0.00632  -0.00103  -0.00736
1.96898
   A45        1.93770   0.00027   0.00368   0.00073   0.00443
1.94213
   A46        1.87017   0.00000   0.00032  -0.00029   0.00001
1.87019
   A47        1.86874  -0.00004   0.00096  -0.00036   0.00061
1.86936
   A48        1.86412   0.00018  -0.00134   0.00022  -0.00111
1.86301
    D1       -0.00055   0.00001  -0.00096   0.00118   0.00023  -
0.00033
```

This journal is © The Royal Society of Chemistry 2014

D2	3.14088	0.00000	-0.00281	0.00112	-0.00169	3.13919
D3	-3.14131	0.00000	0.00042	0.00030	0.00072	-3.14058
D4	0.00013	-0.00001	-0.00143	0.00024	-0.00119	-0.00107
D5	0.00104	0.00000	0.00292	-0.00084	0.00208	0.00312
D6	-3.14116	0.00001	0.00444	-0.00075	0.00369	-3.13746
D7	-3.14139	0.00000	0.00155	0.00004	0.00159	-3.13980
D8	-0.00040	0.00002	0.00307	0.00013	0.00320	0.00281
D9	-0.00085	-0.00001	-0.00369	-0.00010	-0.00380	-0.00465
D10	3.14080	-0.00001	-0.00522	0.00004	-0.00518	3.13562
D11	3.14090	0.00000	-0.00189	-0.00004	-0.00192	3.13897
D12	-0.00064	0.00000	-0.00342	0.00010	-0.00331	-0.00395
D13	0.00174	0.00000	0.00623	-0.00129	0.00495	0.00669
D14	-3.14082	0.00001	0.00190	0.00120	0.00309	-3.13773
D15	-3.13991	0.00000	0.00774	-0.00142	0.00631	-3.13360
D16	0.00071	0.00001	0.00340	0.00106	0.00445	0.00516
D17	-3.13877	-0.00002	0.00700	-0.00278	0.00422	-3.13455
D18	-0.00040	0.00003	0.00403	-0.00059	0.00344	0.00304
D19	0.00288	-0.00002	0.00547	-0.00264	0.00284	0.00572
D20	3.14125	0.00003	0.00250	-0.00045	0.00205	-3.13988
D21	-0.00130	0.00001	-0.00442	0.00165	-0.00277	-0.00407
D22	3.13886	0.00000	-0.00853	0.00176	-0.00676	3.13210
D23	3.14129	0.00000	0.00004	-0.00088	-0.00086	3.14043
D24	-0.00174	0.00000	-0.00407	-0.00078	-0.00485	-0.00659
D25	-0.00505	0.00000	-0.01231	0.00113	-0.01119	-0.01624
D26	3.13875	-0.00001	-0.00929	0.00295	-0.00636	3.13239
D27	3.13552	0.00001	-0.01689	0.00374	-0.01315	3.12237

This journal is © The Royal Society of Chemistry 2014

D28	-0.00386	-0.00001	-0.01387	0.00556	-0.00832	-0.01218
D29	-0.00008	-0.00001	-0.00011	-0.00062	-0.00073	-0.00081
D30	-3.14107	-0.00002	-0.00163	-0.00071	-0.00235	3.13977
D31	-3.14025	0.00000	0.00396	-0.00072	0.00323	-3.13701
D32	0.00195	-0.00002	0.00243	-0.00082	0.00162	0.00357
D33	-0.00208	0.00001	-0.00527	0.00200	-0.00326	-0.00534
D34	3.13896	0.00002	-0.00633	0.00166	-0.00467	3.13428
D35	-3.14045	-0.00003	-0.00230	-0.00019	-0.00248	3.14026
D36	0.00058	-0.00003	-0.00336	-0.00053	-0.00389	-0.00330
D37	0.00583	-0.00001	0.01251	-0.00177	0.01072	0.01655
D38	-3.13369	-0.00004	0.01461	-0.00147	0.01313	-3.12055
D39	-3.13807	0.00001	0.00948	-0.00366	0.00579	-3.13228
D40	0.00561	-0.00001	0.01158	-0.00336	0.00820	0.01380
D41	1.07273	0.00015	0.12165	0.00024	0.12188	1.19461
D42	-3.10317	-0.00013	0.11956	-0.00035	0.11922	-2.98395
D43	-1.00636	-0.00002	0.11611	-0.00025	0.11586	-0.89050
D44	-2.06659	0.00013	0.12470	0.00210	0.12679	-1.93981
D45	0.04069	-0.00015	0.12261	0.00151	0.12413	0.16482
D46	2.13750	-0.00004	0.11915	0.00161	0.12077	2.25827
D47	-0.00233	0.00000	-0.00382	0.00024	-0.00358	-0.00591
D48	3.13982	0.00000	-0.00277	0.00058	-0.00219	3.13762
D49	3.13732	0.00003	-0.00579	-0.00004	-0.00584	3.13148
D50	-0.00372	0.00002	-0.00475	0.00030	-0.00445	-0.00817
D51	-3.14054	0.00000	0.00100	-0.00109	-0.00009	-3.14063
D52	0.00403	-0.00002	0.00401	-0.00061	0.00340	0.00743
D53	0.00308	-0.00003	0.00304	-0.00080	0.00225	0.00534

```
   D54       -3.13553  -0.00004   0.00605  -0.00031   0.00574  -
3.12979
   D55        0.00161   0.00000   0.00293   0.00039   0.00333
0.00493
   D56       -3.13931   0.00000   0.00409   0.00102   0.00513  -
3.13418
   D57       -3.14055   0.00000   0.00188   0.00005   0.00192  -
3.13862
   D58        0.00172   0.00000   0.00304   0.00068   0.00372
0.00545
   D59        0.00110  -0.00002   0.00061  -0.00118  -0.00057
0.00053
   D60        3.14124   0.00000  -0.00004  -0.00093  -0.00097
3.14027
   D61       -3.13980  -0.00002   0.00180  -0.00053   0.00127  -
3.13852
   D62        0.00034   0.00000   0.00115  -0.00028   0.00087
0.00121
   D63       -0.00183   0.00001  -0.00244   0.00069  -0.00175  -
0.00358
   D64        3.13977   0.00000  -0.00370   0.00045  -0.00325
3.13652
   D65        3.14121  -0.00001  -0.00179   0.00044  -0.00135
3.13986
   D66       -0.00038  -0.00002  -0.00306   0.00021  -0.00285  -
0.00323
   D67       -0.00036   0.00002   0.00052   0.00032   0.00084
0.00048
   D68        3.13831   0.00003  -0.00247  -0.00015  -0.00261
3.13570
   D69        3.14123   0.00003   0.00179   0.00056   0.00234  -
3.13961
   D70       -0.00329   0.00004  -0.00120   0.00008  -0.00111  -
0.00440
         Item               Value     Threshold  Converged?
 Maximum Force            0.001432     0.000450     NO
 RMS     Force            0.000226     0.000300     YES
 Maximum Displacement     0.257991     0.001800     NO
 RMS     Displacement     0.035369     0.001200     NO
 Predicted change in Energy=-2.009339D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793211   -5.421502    0.014412
      2          6           0       -3.422656   -5.393263    0.000836
      3          6           0       -2.706600   -4.154351   -0.011519
```

4	6	0	-3.441214	-2.909444	-0.015511
5	6	0	-4.873270	-2.991234	0.001857
6	6	0	-5.525626	-4.199895	0.016753
7	6	0	-1.308390	-4.125617	-0.018218
8	6	0	-2.747879	-1.672361	-0.032456
9	6	0	-1.330378	-1.663150	-0.025447
10	6	0	-0.604499	-2.918244	-0.021886
11	6	0	0.827375	-2.905415	-0.019750
12	1	0	1.348464	-3.860411	-0.019938
13	6	0	1.528884	-1.728933	-0.014628
14	6	0	0.826113	-0.489658	-0.010679
15	6	0	-0.546145	-0.459838	-0.016164
16	1	0	-0.755965	-5.063527	-0.016828
17	1	0	-5.324152	-6.369831	0.024646
18	1	0	-2.850225	-6.318418	0.001137
19	1	0	-5.460294	-2.079491	0.008460
20	1	0	-6.612312	-4.226621	0.031442
21	1	0	2.615716	-1.734736	-0.011819
22	1	0	1.384494	0.443034	-0.001816
23	1	0	-1.040481	0.504450	-0.007253
24	6	0	-3.547942	-0.386799	-0.048404
25	1	0	-4.077878	-0.232102	0.901242
26	1	0	-2.928858	0.494291	-0.218380
27	1	0	-4.304499	-0.398947	-0.841575

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370914	0.000000			
3	C	2.441371	1.431010	0.000000		
4	C	2.852933	2.483942	1.445499	0.000000	
5	C	2.431619	2.806069	2.459163	1.434495	0.000000
6	C	1.424346	2.418029	2.819536	2.451749	1.373554
7	C	3.718113	2.465240	1.398521	2.455204	3.741069
8	C	4.271023	3.781738	2.482422	1.418230	2.501577
9	C	5.110579	4.276922	2.846096	2.451322	3.783733
10	C	4.879850	3.750766	2.438626	2.836736	4.269461
11	C	6.158153	4.924690	3.748184	4.268593	5.701332
12	H	6.337062	5.011352	4.065712	4.883173	6.282191
13	C	7.321530	6.159975	4.880777	5.108374	6.525431
14	C	7.476665	6.488259	5.090190	4.905657	6.224227
15	C	6.531203	5.710803	4.279838	3.792360	5.013213
16	H	4.053206	2.687057	2.152116	3.442476	4.609441
17	H	1.086890	2.137742	3.429466	3.939714	3.408626
18	H	2.140054	1.087929	2.168865	3.459863	3.893953
19	H	3.407943	3.890130	3.447938	2.183136	1.084397
20	H	2.176501	3.396454	3.906617	3.434097	2.133383
21	H	8.275575	7.060234	5.846502	6.169794	7.593674
22	H	8.518045	7.561154	6.154111	5.875947	7.138194
23	H	7.014297	6.360648	4.947767	4.173519	5.187501
24	C	5.186799	5.008273	3.860527	2.525116	2.922688
25	H	5.313007	5.279927	4.254125	2.900679	3.009045

This journal is © The Royal Society of Chemistry 2014

26	H	6.206981	5.912290	4.658547	3.448054	3.997265
27	H	5.118361	5.141060	4.164773	2.780331	2.784750
		6	7	8	9	10
6	C	0.000000				
7	C	4.218035	0.000000			
8	C	3.755892	2.844433	0.000000		
9	C	4.902750	2.462576	1.417549	0.000000	
10	C	5.085431	1.397579	2.479196	1.449887	0.000000
11	C	6.483643	2.459753	3.781934	2.489810	1.431933
12	H	6.882565	2.670058	4.644109	3.464705	2.168351
13	C	7.474807	3.714058	4.277175	2.860039	2.442506
14	C	7.356031	4.216201	3.764662	2.455148	2.818652
15	C	6.227707	3.744189	2.513585	1.436338	2.459104
16	H	4.847335	1.088508	3.932934	3.448563	2.150630
17	H	2.179284	4.600509	5.357860	6.172972	5.847286
18	H	3.412646	2.680673	4.647306	4.897159	4.074924
19	H	2.121427	4.628786	2.743105	4.150988	4.927796
20	H	1.087114	5.305116	4.632728	5.871409	6.148863
21	H	8.506425	4.595101	5.363998	3.946767	3.430827
22	H	8.325076	5.303250	4.642450	3.436146	3.905724
23	H	6.499843	4.637825	2.766650	2.186975	3.450381
24	C	4.295949	4.358356	1.514274	2.558748	3.882367
25	H	4.315284	4.865689	2.171413	3.233482	4.486857
26	H	5.369718	4.899952	2.182132	2.692009	4.133600
27	H	4.083514	4.852078	2.167792	3.333117	4.550686
		11	12	13	14	15
11	C	0.000000				
12	H	1.087912	0.000000			
13	C	1.369763	2.139107	0.000000		
14	C	2.415774	3.410999	1.424677	0.000000	
15	C	2.804891	3.892744	2.432355	1.372593	0.000000
16	H	2.676643	2.424070	4.042283	4.839761	4.608467
17	H	7.060130	7.129024	8.276689	8.509021	7.599936
18	H	5.017347	4.865309	6.343518	6.891302	6.295399
19	H	6.341745	7.037874	6.998002	6.484354	5.174238
20	H	7.556265	7.969360	8.515846	8.324472	7.140679
21	H	2.137456	2.474770	1.086851	2.180115	3.409215
22	H	3.394527	4.303634	2.176799	1.087098	2.131373
23	H	3.887959	4.975865	3.404364	2.114813	1.083651
24	C	5.048529	6.003464	5.251345	4.375426	3.002858
25	H	5.661831	6.592298	5.874955	4.994703	3.656040
26	H	5.070181	6.107233	4.985549	3.887300	2.574602
27	H	5.770087	6.679282	6.039955	5.198249	3.848407
		16	17	18	19	20
16	H	0.000000				
17	H	4.751472	0.000000			
18	H	2.441516	2.474573	0.000000		
19	H	5.570981	4.292530	4.978054	0.000000	
20	H	5.916041	2.500550	4.304629	2.436769	0.000000
21	H	4.738049	9.193853	7.133500	8.083391	9.558654
22	H	5.907961	9.561473	7.978101	7.294817	9.260437
23	H	5.575250	8.099790	7.058809	5.119741	7.309571

24	C	5.446826	6.241549	5.972719	2.554512	4.913347
25	H	5.934697	6.324029	6.273800	2.474062	4.809999
26	H	5.970881	7.274109	6.816698	3.617178	5.993101
27	H	5.918666	6.118945	6.153472	2.209672	4.554037

		21	22	23	24	25
21	H	0.000000				
22	H	2.501737	0.000000			
23	H	4.287395	2.425759	0.000000		
24	C	6.309433	5.001971	2.661461	0.000000	
25	H	6.920678	5.577528	3.254788	1.098449	0.000000
26	H	5.979425	4.319089	1.900169	1.090172	1.761092
27	H	7.096633	5.811950	3.487984	1.096197	1.765391

		26	27
26	H	0.000000	
27	H	1.754604	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.653963	-1.002867	0.008742
2	6	0	-2.454578	-1.666741	-0.003531
3	6	0	-1.213116	-0.955019	-0.007606
4	6	0	-1.223104	0.490442	-0.004476
5	6	0	-2.502579	1.138879	0.011207
6	6	0	-3.673774	0.421310	0.018064
7	6	0	0.010405	-1.632389	-0.012977
8	6	0	-0.002190	1.212016	-0.013170
9	6	0	1.228155	0.508008	-0.004938
10	6	0	1.225474	-0.941872	-0.008571
11	6	0	2.470083	-1.649946	-0.005178
12	1	0	2.441049	-2.737455	-0.010864
13	6	0	3.667544	-0.984989	0.007824
14	6	0	3.682234	0.439570	0.018887
15	6	0	2.510609	1.154597	0.012459
16	1	0	0.017043	-2.720869	-0.016954
17	1	0	-4.589403	-1.556282	0.012652
18	1	0	-2.424230	-2.754235	-0.008501
19	1	0	-2.552309	2.222071	0.022986
20	1	0	-4.626936	0.943914	0.031692
21	1	0	4.604428	-1.535880	0.011491
22	1	0	4.633475	0.965587	0.033999
23	1	0	2.567410	2.236662	0.026948
24	6	0	-0.048307	2.725563	-0.021797
25	1	0	-0.432497	3.120786	0.928355
26	1	0	0.930193	3.177357	-0.185791

```
     27          1           0       -0.705583    3.098968   -0.815651
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3939540      0.4478427
0.3396780
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9026984884 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
```

```
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860659572     A.U. after   12 cycles
             Convg  =    0.1588D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000048886    0.000026562   -0.000020284
      2        6          -0.000024855    0.000017266    0.000023366
      3        6          -0.000060569    0.000076743    0.000027700
      4        6           0.000026897   -0.000057239   -0.000027300
      5        6           0.000103803    0.000082844    0.000019537
      6        6           0.000018211    0.000033381    0.000038182
      7        6           0.000040126    0.000044469   -0.000024472
      8        6           0.000136619   -0.000066122   -0.000087455
      9        6          -0.000081690    0.000101846    0.000013544
     10        6          -0.000029798   -0.000033583    0.000017325
     11        6           0.000057765    0.000068217    0.000011622
     12        1           0.000005021   -0.000010367   -0.000004600
     13        6          -0.000040163   -0.000114395   -0.000015720
     14        6          -0.000166044    0.000030902    0.000023697
     15        6           0.000337711   -0.000084629   -0.000013665
     16        1           0.000004808   -0.000014262   -0.000006929
     17        1          -0.000024143   -0.000016010    0.000003711
     18        1           0.000005629   -0.000012215   -0.000005753
     19        1           0.000039176    0.000222253    0.000031383
     20        1          -0.000025791   -0.000017225   -0.000001085
     21        1           0.000030525    0.000009966    0.000000056
     22        1           0.000025296    0.000012543   -0.000005537
     23        1           0.000228704   -0.000013559    0.000040588
     24        6          -0.000057753    0.000193182   -0.000009358
     25        1          -0.000163705   -0.000150660    0.000097734
     26        1          -0.000462304   -0.000233526   -0.000035261
     27        1           0.000027638   -0.000096381   -0.000091025
```

This journal is © The Royal Society of Chemistry 2014

```
 ----------------------------------------------------------------------
 Cartesian Forces:  Max     0.000462304 RMS     0.000097306


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.001436673 RMS     0.000220529
 Search for a local minimum.
 Step number  43 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   21   28   29   30
31
                                                     32   33   35   34
36
                                                     37   38   39   40
41
                                                     42   43
 DE=  2.09D-05 DEPred=-2.01D-05 R=-1.04D+00
 Trust test=-1.04D+00 RLast= 3.01D-01 DXMaxT set to 2.00D-01
     Eigenvalues ---    0.00001   0.00738   0.01058   0.01559
0.01684
     Eigenvalues ---    0.01765   0.01806   0.01826   0.01855
0.01929
     Eigenvalues ---    0.01972   0.01976   0.02007   0.02068
0.02095
     Eigenvalues ---    0.02107   0.02140   0.02145   0.02219
0.02225
     Eigenvalues ---    0.02318   0.02345   0.06002   0.06276
0.08023
     Eigenvalues ---    0.11408   0.12238   0.15490   0.15759
0.15978
     Eigenvalues ---    0.16000   0.16002   0.16003   0.16013
0.16042
     Eigenvalues ---    0.16516   0.17336   0.21025   0.22007
0.22551
     Eigenvalues ---    0.22668   0.22898   0.24028   0.24546
0.24615
     Eigenvalues ---    0.25178   0.27330   0.31030   0.32263
0.33217
     Eigenvalues ---    0.33590   0.33630   0.33652   0.33682
0.33682
     Eigenvalues ---    0.33856   0.34157   0.34675   0.36233
0.37501
     Eigenvalues ---    0.37641   0.37842   0.38259   0.39472
0.40256
     Eigenvalues ---    0.40511   0.40890   0.43004   0.44566
0.45968
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.47919   0.49683   0.49932   0.51243
0.52081
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   1.18D-05 Eigenvector:
                          D45       D44       D46       D42       D41
   1                    0.42185   0.40536   0.39963   0.39679
0.38030
                          D43       D27       D38       D37       D25
   1                    0.37457  -0.08767   0.08289   0.07023  -
0.06494
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    43   42   41   40
39
 RFO step:  Lambda=-1.28297658D-05.
 DIIS coeffs:      0.46949      0.65370      0.04964     -0.14418
-0.02865
 Maximum step size (   0.200) exceeded in Quadratic search.
    -- Step size scaled by   0.908
 Iteration  1 RMS(Cart)=  0.02334544 RMS(Int)=  0.00085509
 Iteration  2 RMS(Cart)=  0.00088697 RMS(Int)=  0.00000172
 Iteration  3 RMS(Cart)=  0.00000101 RMS(Int)=  0.00000153
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000153
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
```

R1	2.59065	0.00004	0.00023	-0.00005	0.00018
2.59084					
R2	2.69162	0.00006	-0.00012	0.00013	0.00001
2.69163					
R3	2.05393	0.00003	0.00012	-0.00007	0.00005
2.05397					
R4	2.70422	0.00000	-0.00013	0.00001	-0.00012
2.70410					
R5	2.05589	0.00001	0.00003	-0.00003	0.00000
2.05589					
R6	2.73160	-0.00030	-0.00100	0.00001	-0.00099
2.73061					
R7	2.64282	-0.00007	-0.00002	0.00015	0.00013
2.64295					
R8	2.71080	-0.00022	-0.00045	0.00011	-0.00034
2.71046					
R9	2.68007	-0.00043	-0.00023	0.00023	-0.00001
2.68006					
R10	2.59564	-0.00002	0.00004	0.00003	0.00007
2.59571					
R11	2.04921	0.00017	0.00025	-0.00005	0.00019
2.04941					
R12	2.05435	0.00003	0.00019	-0.00014	0.00005
2.05439					
R13	2.64104	0.00002	-0.00018	0.00001	-0.00017
2.64087					
R14	2.05698	0.00001	0.00007	-0.00006	0.00001
2.05699					
R15	2.67878	0.00048	-0.00027	0.00000	-0.00027
2.67851					
R16	2.86156	0.00010	0.00000	0.00022	0.00022
2.86178					
R17	2.73989	0.00026	0.00071	0.00015	0.00086
2.74075					
R18	2.71428	0.00026	0.00005	0.00024	0.00029
2.71458					
R19	2.70596	0.00002	0.00018	0.00006	0.00024
2.70620					
R20	2.05586	0.00001	0.00002	-0.00003	-0.00001
2.05585					
R21	2.58848	-0.00017	-0.00018	-0.00010	-0.00027
2.58820					
R22	2.69225	-0.00005	-0.00005	0.00018	0.00013
2.69238					
R23	2.05385	0.00003	0.00011	-0.00008	0.00003
2.05388					
R24	2.59382	-0.00011	-0.00034	-0.00001	-0.00034
2.59348					
R25	2.05432	0.00002	0.00018	-0.00014	0.00004
2.05435					
R26	2.04780	-0.00012	0.00000	-0.00008	-0.00009
2.04772					

This journal is © The Royal Society of Chemistry 2014

R27	2.07577	0.00014	-0.00050	-0.00017	-0.00067
2.07510					
R28	2.06013	-0.00045	-0.00103	-0.00008	-0.00112
2.05901					
R29	2.07151	0.00005	0.00160	0.00002	0.00162
2.07313					
A1	2.09027	0.00002	0.00027	0.00006	0.00033
2.09061					
A2	2.10184	0.00000	0.00010	-0.00027	-0.00016
2.10168					
A3	2.09107	-0.00003	-0.00037	0.00021	-0.00017
2.09090					
A4	2.11551	-0.00005	-0.00023	-0.00001	-0.00024
2.11527					
A5	2.10425	0.00002	0.00010	-0.00019	-0.00009
2.10416					
A6	2.06343	0.00002	0.00013	0.00019	0.00033
2.06375					
A7	2.08443	-0.00008	-0.00025	-0.00003	-0.00028
2.08415					
A8	2.11543	0.00019	0.00101	0.00000	0.00101
2.11644					
A9	2.08333	-0.00011	-0.00076	0.00003	-0.00074
2.08259					
A10	2.04677	0.00024	0.00083	0.00008	0.00090
2.04768					
A11	2.09764	0.00034	0.00105	-0.00005	0.00101
2.09865					
A12	2.13877	-0.00057	-0.00188	-0.00003	-0.00191
2.13686					
A13	2.12285	-0.00007	-0.00036	-0.00008	-0.00044
2.12241					
A14	2.08582	-0.00012	-0.00031	-0.00019	-0.00050
2.08531					
A15	2.07451	0.00019	0.00068	0.00027	0.00095
2.07546					
A16	2.10652	-0.00006	-0.00024	-0.00003	-0.00027
2.10625					
A17	2.08627	0.00001	-0.00015	0.00010	-0.00004
2.08622					
A18	2.09040	0.00005	0.00038	-0.00008	0.00031
2.09071					
A19	2.11917	0.00001	0.00002	-0.00001	0.00002
2.11919					
A20	2.08252	-0.00001	0.00012	0.00000	0.00011
2.08264					
A21	2.08148	0.00000	-0.00014	0.00001	-0.00013
2.08136					
A22	2.08802	0.00001	0.00018	0.00002	0.00021
2.08822					
A23	2.07414	-0.00144	-0.00551	-0.00008	-0.00559
2.06855					

A24	2.12101	0.00143	0.00534	0.00006	0.00540	2.12640
A25	2.08865	-0.00038	-0.00113	-0.00002	-0.00115	2.08750
A26	2.15490	0.00071	0.00188	0.00000	0.00188	2.15678
A27	2.03963	-0.00033	-0.00075	0.00002	-0.00073	2.03890
A28	2.08943	0.00014	0.00073	0.00002	0.00075	2.09018
A29	2.10757	-0.00026	-0.00094	0.00003	-0.00090	2.10666
A30	2.08618	0.00012	0.00021	-0.00005	0.00016	2.08634
A31	2.06133	-0.00002	-0.00031	0.00018	-0.00013	2.06120
A32	2.11743	0.00005	0.00016	0.00002	0.00018	2.11762
A33	2.10442	-0.00002	0.00015	-0.00020	-0.00005	2.10437
A34	2.08806	-0.00004	-0.00030	0.00008	-0.00022	2.08784
A35	2.10314	0.00003	0.00043	-0.00028	0.00015	2.10329
A36	2.09199	0.00001	-0.00012	0.00020	0.00007	2.09206
A37	2.10837	0.00007	0.00021	-0.00004	0.00017	2.10854
A38	2.08629	-0.00005	-0.00011	0.00007	-0.00004	2.08625
A39	2.08853	-0.00002	-0.00010	-0.00004	-0.00014	2.08839
A40	2.12667	0.00012	0.00049	-0.00004	0.00045	2.12712
A41	2.09032	0.00014	0.00076	-0.00018	0.00059	2.09091
A42	2.06617	-0.00026	-0.00124	0.00022	-0.00103	2.06515
A43	1.94481	-0.00016	-0.00227	-0.00012	-0.00239	1.94242
A44	1.96898	0.00045	0.00447	-0.00046	0.00400	1.97299
A45	1.94213	-0.00027	-0.00188	-0.00028	-0.00216	1.93997
A46	1.87019	0.00003	-0.00044	-0.00014	-0.00058	1.86961
A47	1.86936	0.00007	-0.00068	0.00007	-0.00061	1.86875
A48	1.86301	-0.00011	0.00073	0.00100	0.00173	1.86473
D1	-0.00033	-0.00001	-0.00014	0.00019	0.00005	-0.00027

This journal is © The Royal Society of Chemistry 2014

D2	3.13919	-0.00001	0.00124	-0.00004	0.00120	3.14039
D3	-3.14058	0.00000	-0.00064	0.00006	-0.00058	-3.14117
D4	-0.00107	0.00000	0.00075	-0.00018	0.00057	-0.00050
D5	0.00312	0.00002	-0.00168	0.00018	-0.00150	0.00162
D6	-3.13746	0.00001	-0.00261	0.00048	-0.00212	-3.13958
D7	-3.13980	0.00001	-0.00118	0.00031	-0.00087	-3.14067
D8	0.00281	0.00000	-0.00211	0.00062	-0.00149	0.00131
D9	-0.00465	-0.00001	0.00276	-0.00038	0.00239	-0.00226
D10	3.13562	-0.00001	0.00360	-0.00043	0.00317	3.13878
D11	3.13897	-0.00001	0.00141	-0.00015	0.00126	3.14024
D12	-0.00395	-0.00001	0.00224	-0.00020	0.00204	-0.00191
D13	0.00669	0.00002	-0.00351	0.00020	-0.00331	0.00338
D14	-3.13773	0.00000	-0.00207	0.00017	-0.00189	-3.13962
D15	-3.13360	0.00002	-0.00432	0.00025	-0.00408	-3.13767
D16	0.00516	0.00000	-0.00288	0.00023	-0.00266	0.00251
D17	-3.13455	0.00004	-0.00338	0.00023	-0.00315	-3.13770
D18	0.00304	0.00001	-0.00263	0.00103	-0.00160	0.00144
D19	0.00572	0.00004	-0.00255	0.00018	-0.00237	0.00334
D20	-3.13988	0.00001	-0.00180	0.00098	-0.00082	-3.14070
D21	-0.00407	-0.00001	0.00179	0.00017	0.00195	-0.00212
D22	3.13210	-0.00003	0.00463	-0.00003	0.00460	3.13670
D23	3.14043	0.00001	0.00031	0.00019	0.00049	3.14092
D24	-0.00659	-0.00001	0.00315	-0.00001	0.00315	-0.00344
D25	-0.01624	-0.00004	0.00798	-0.00060	0.00738	-0.00886
D26	3.13239	-0.00004	0.00521	-0.00109	0.00411	3.13650
D27	3.12237	-0.00007	0.00950	-0.00063	0.00888	3.13124

This journal is © The Royal Society of Chemistry 2014

D28	-0.01218	-0.00006	0.00673	-0.00112	0.00561	-0.00658
D29	-0.00081	-0.00001	0.00080	-0.00036	0.00044	-0.00037
D30	3.13977	0.00000	0.00173	-0.00067	0.00107	3.14084
D31	-3.13701	0.00001	-0.00203	-0.00016	-0.00219	-3.13920
D32	0.00357	0.00002	-0.00110	-0.00047	-0.00157	0.00200
D33	-0.00534	-0.00002	0.00278	-0.00020	0.00259	-0.00275
D34	3.13428	-0.00003	0.00354	-0.00019	0.00335	3.13764
D35	3.14026	0.00000	0.00203	-0.00100	0.00103	3.14129
D36	-0.00330	0.00000	0.00279	-0.00099	0.00180	-0.00151
D37	0.01655	0.00005	-0.00772	0.00058	-0.00714	0.00941
D38	-3.12055	0.00005	-0.00923	0.00024	-0.00899	-3.12955
D39	-3.13228	0.00003	-0.00488	0.00108	-0.00381	-3.13608
D40	0.01380	0.00003	-0.00640	0.00074	-0.00566	0.00814
D41	1.19461	-0.00018	-0.07540	-0.00518	-0.08058	1.11402
D42	-2.98395	0.00005	-0.07447	-0.00576	-0.08024	-3.06419
D43	-0.89050	0.00003	-0.07179	-0.00500	-0.07678	-0.96728
D44	-1.93981	-0.00017	-0.07822	-0.00568	-0.08390	-2.02371
D45	0.16482	0.00006	-0.07729	-0.00627	-0.08356	0.08126
D46	2.25827	0.00004	-0.07461	-0.00550	-0.08010	2.17817
D47	-0.00591	-0.00002	0.00240	-0.00018	0.00222	-0.00370
D48	3.13762	-0.00001	0.00165	-0.00019	0.00146	3.13909
D49	3.13148	-0.00002	0.00382	0.00013	0.00395	3.13544
D50	-0.00817	-0.00001	0.00307	0.00013	0.00320	-0.00496
D51	-3.14063	0.00000	0.00009	-0.00014	-0.00006	-3.14068
D52	0.00743	0.00002	-0.00251	-0.00017	-0.00268	0.00475
D53	0.00534	0.00001	-0.00139	-0.00047	-0.00186	0.00348

```
   D54       -3.12979   0.00003  -0.00398  -0.00051  -0.00449  -
3.13428
   D55        0.00493   0.00001  -0.00204   0.00009  -0.00195
0.00298
   D56       -3.13418   0.00001  -0.00338   0.00025  -0.00313  -
3.13731
   D57       -3.13862   0.00001  -0.00129   0.00010  -0.00119  -
3.13981
   D58        0.00545   0.00001  -0.00262   0.00026  -0.00237
0.00308
   D59        0.00053   0.00001   0.00033  -0.00031   0.00002
0.00056
   D60        3.14027   0.00000   0.00070  -0.00004   0.00066
3.14092
   D61       -3.13852   0.00001  -0.00104  -0.00015  -0.00118  -
3.13971
   D62        0.00121   0.00000  -0.00067   0.00012  -0.00055
0.00066
   D63       -0.00358  -0.00001   0.00144  -0.00004   0.00141  -
0.00217
   D64        3.13652  -0.00001   0.00234  -0.00027   0.00206
3.13858
   D65        3.13986   0.00000   0.00108  -0.00030   0.00077
3.14064
   D66       -0.00323   0.00000   0.00197  -0.00054   0.00143  -
0.00180
   D67        0.00048   0.00001  -0.00087   0.00044  -0.00043
0.00005
   D68        3.13570  -0.00001   0.00169   0.00047   0.00216
3.13786
   D69       -3.13961   0.00000  -0.00176   0.00067  -0.00109  -
3.14070
   D70       -0.00440  -0.00002   0.00080   0.00070   0.00151  -
0.00289
         Item               Value     Threshold  Converged?
 Maximum Force            0.001437     0.000450     NO
 RMS     Force            0.000221     0.000300     YES
 Maximum Displacement     0.172873     0.001800     NO
 RMS     Displacement     0.023349     0.001200     NO
 Predicted change in Energy=-2.017463D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793457   -5.418674    0.015813
      2          6           0       -3.422735   -5.391999    0.006679
      3          6           0       -2.705573   -4.153801   -0.005704
```

This journal is © The Royal Society of Chemistry 2014

4	6	0	-3.439133	-2.908886	-0.011485
5	6	0	-4.871190	-2.988498	-0.000026
6	6	0	-5.524906	-4.196482	0.013344
7	6	0	-1.307295	-4.124926	-0.011670
8	6	0	-2.746227	-1.671536	-0.026163
9	6	0	-1.328855	-1.661627	-0.024230
10	6	0	-0.603566	-2.917580	-0.019122
11	6	0	0.828445	-2.905921	-0.020294
12	1	0	1.348627	-3.861404	-0.018093
13	6	0	1.531060	-1.730259	-0.022550
14	6	0	0.829226	-0.490368	-0.023078
15	6	0	-0.542832	-0.459262	-0.023914
16	1	0	-0.754660	-5.062713	-0.008163
17	1	0	-5.325360	-6.366497	0.025581
18	1	0	-2.851441	-6.317852	0.009560
19	1	0	-5.456480	-2.075495	0.000706
20	1	0	-6.611696	-4.222384	0.022515
21	1	0	2.617908	-1.736983	-0.022792
22	1	0	1.388396	0.441915	-0.022021
23	1	0	-1.035210	0.506013	-0.020732
24	6	0	-3.553962	-0.390606	-0.038553
25	1	0	-4.146665	-0.284051	0.879687
26	1	0	-2.936016	0.502438	-0.126899
27	1	0	-4.257833	-0.374579	-0.879880

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.371011	0.000000			
3	C	2.441234	1.430947	0.000000		
4	C	2.852013	2.483233	1.444976	0.000000	
5	C	2.431471	2.806222	2.459239	1.434314	0.000000
6	C	1.424352	2.418352	2.819720	2.451320	1.373590
7	C	3.718584	2.465948	1.398590	2.454279	3.740716
8	C	4.270123	3.781611	2.482681	1.418227	2.500107
9	C	5.110819	4.277962	2.847214	2.451344	3.782764
10	C	4.879741	3.751150	2.438617	2.835590	4.268255
11	C	6.158004	4.924819	3.747893	4.267588	5.700269
12	H	6.336516	5.010912	4.064750	4.881596	6.280797
13	C	7.321571	6.160299	4.880871	5.108043	6.524759
14	C	7.476916	6.488917	5.090761	4.905940	6.223819
15	C	6.531857	5.711976	4.281051	3.793332	5.013211
16	H	4.054524	2.688359	2.152252	3.441711	4.609583
17	H	1.086914	2.137752	3.429327	3.938819	3.408490
18	H	2.140090	1.087929	2.169015	3.459317	3.894108
19	H	3.408325	3.890418	3.447736	2.182746	1.084500
20	H	2.176499	3.396722	3.906827	3.433889	2.133623
21	H	8.275547	7.060410	5.846431	6.169378	7.592984
22	H	8.518406	7.561902	6.154791	5.876479	7.137971
23	H	7.016243	6.362984	4.950172	4.176178	5.189101
24	C	5.178878	5.003319	3.857782	2.521042	2.913008
25	H	5.246806	5.232336	4.223224	2.860865	2.934768

This journal is © The Royal Society of Chemistry 2014

26	H	6.207256	5.916006	4.663513	3.450156	3.993448
27	H	5.150928	5.163126	4.178063	2.801266	2.825406
		6	7	8	9	10
6	C	0.000000				
7	C	4.218292	0.000000			
8	C	3.754726	2.844268	0.000000		
9	C	4.902422	2.463425	1.417408	0.000000	
10	C	5.084901	1.397488	2.478643	1.450341	0.000000
11	C	6.483190	2.459153	3.781802	2.490427	1.432060
12	H	6.881767	2.668971	4.643642	3.465251	2.168378
13	C	7.474637	3.713598	4.277692	2.860739	2.442617
14	C	7.356058	4.216025	3.765506	2.455435	2.818558
15	C	6.228102	3.744549	2.514868	1.436494	2.459073
16	H	4.848305	1.088513	3.932778	3.449253	2.150475
17	H	2.179204	4.601182	5.356982	6.173356	5.847423
18	H	3.412864	2.682119	4.647644	4.898963	4.076225
19	H	2.122128	4.627749	2.740324	4.148397	4.925472
20	H	1.087138	5.305407	4.631528	5.870952	6.148323
21	H	8.506225	4.594520	5.364536	3.947483	3.430995
22	H	8.325246	5.303102	4.643469	3.436327	3.905654
23	H	6.501691	4.638934	2.769355	2.187442	3.450697
24	C	4.286258	4.358140	1.514388	2.562577	3.884689
25	H	4.237595	4.858895	2.169540	3.264174	4.505206
26	H	5.366737	4.906986	2.184567	2.697533	4.141070
27	H	4.124350	4.850213	2.166999	3.311728	4.534471
		11	12	13	14	15
11	C	0.000000				
12	H	1.087907	0.000000			
13	C	1.369618	2.138943	0.000000		
14	C	2.415555	3.410819	1.424747	0.000000	
15	C	2.804738	3.892585	2.432379	1.372411	0.000000
16	H	2.675467	2.422201	4.041036	4.838932	4.608349
17	H	7.060241	7.128779	8.276926	8.509417	7.600687
18	H	5.018339	4.865745	6.344553	6.892601	6.297132
19	H	6.339585	7.035574	6.996103	6.482538	5.172693
20	H	7.555833	7.968607	8.515704	8.324503	7.141033
21	H	2.137429	2.474724	1.086869	2.180237	3.409231
22	H	3.394342	4.303504	2.176854	1.087117	2.131142
23	H	3.887738	4.975642	3.403919	2.113978	1.083606
24	C	5.052983	6.006849	5.258553	4.384350	3.011947
25	H	5.695251	6.618285	5.928078	5.061328	3.719516
26	H	5.079316	6.116627	4.995057	3.895316	2.581240
27	H	5.746025	6.658304	6.007010	5.160008	3.813277
		16	17	18	19	20
16	H	0.000000				
17	H	4.753134	0.000000			
18	H	2.443804	2.474449	0.000000		
19	H	5.570517	4.293077	4.978343	0.000000	
20	H	5.917091	2.500378	4.304727	2.438060	0.000000
21	H	4.736551	9.194033	7.134367	8.081516	9.558498
22	H	5.907098	9.561969	7.979453	7.293161	9.260624
23	H	5.575802	8.101784	7.061497	5.119792	7.311416

This journal is © The Royal Society of Chemistry 2014

24	C	5.446614	6.233236	5.968928	2.541647	4.902652
25	H	5.927021	6.254196	6.232293	2.386942	4.724573
26	H	5.978572	7.274234	6.822179	3.607598	5.988063
27	H	5.916985	6.153255	6.171834	2.259491	4.600065

		21	22	23	24	25
21	H	0.000000				
22	H	2.501859	0.000000			
23	H	4.286760	2.424454	0.000000		
24	C	6.317037	5.012012	2.673640	0.000000	
25	H	6.977459	5.654821	3.334082	1.098097	0.000000
26	H	5.989317	4.326107	1.903772	1.089582	1.759958
27	H	7.061626	5.769098	3.449475	1.097052	1.765398

		26	27
26	H	0.000000	
27	H	1.755944	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.652385	-1.004801	0.004975
2	6	0	-2.452838	-1.668667	-0.001462
3	6	0	-1.211642	-0.956603	-0.003920
4	6	0	-1.222472	0.488332	-0.002388
5	6	0	-2.501636	1.137121	0.005893
6	6	0	-3.672793	0.419397	0.009664
7	6	0	0.012837	-1.632394	-0.007123
8	6	0	-0.002680	1.211832	-0.007191
9	6	0	1.228776	0.510020	-0.002592
10	6	0	1.226920	-0.940318	-0.004889
11	6	0	2.471937	-1.647937	-0.003355
12	1	0	2.443197	-2.735458	-0.006845
13	6	0	3.669153	-0.982747	0.003852
14	6	0	3.683231	0.441914	0.010660
15	6	0	2.511537	1.156501	0.007526
16	1	0	0.021041	-2.720874	-0.009124
17	1	0	-4.587728	-1.558435	0.007176
18	1	0	-2.422503	-2.756171	-0.003972
19	1	0	-2.550541	2.220500	0.011901
20	1	0	-4.626257	0.941627	0.016663
21	1	0	4.606270	-1.533284	0.005555
22	1	0	4.634327	0.968380	0.019225
23	1	0	2.569216	2.238533	0.016518
24	6	0	-0.059612	2.725141	-0.012154
25	1	0	-0.523753	3.109721	0.905718
26	1	0	0.923132	3.188651	-0.093155

```
     27          1           0       -0.656397    3.096075   -0.854637
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3942128      0.4478361
0.3396791
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9195241525 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
```

```
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860686377     A.U. after   11 cycles
             Convg  =    0.6112D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000033029    0.000000033   -0.000006453
      2        6          -0.000027951    0.000015758    0.000004178
      3        6          -0.000037603    0.000020305    0.000009147
      4        6          -0.000000331   -0.000006644   -0.000025061
      5        6           0.000041867    0.000007820    0.000004272
      6        6           0.000010208    0.000010298    0.000014198
      7        6           0.000014414    0.000001403    0.000002436
      8        6           0.000012528   -0.000020589    0.000031180
      9        6          -0.000022380    0.000017568    0.000021306
     10        6           0.000010420    0.000008378    0.000011059
     11        6           0.000019792    0.000055732    0.000000787
     12        1          -0.000002275   -0.000017508    0.000000236
     13        6          -0.000023490   -0.000058836   -0.000007972
     14        6          -0.000051605    0.000007109    0.000009984
     15        6           0.000086662   -0.000018195   -0.000016109
     16        1           0.000001860   -0.000011981   -0.000015753
     17        1          -0.000015877   -0.000006470    0.000002069
     18        1           0.000014456   -0.000007405   -0.000001592
     19        1           0.000001155    0.000061905    0.000012751
     20        1          -0.000010197   -0.000011910    0.000007435
     21        1           0.000016374    0.000010429   -0.000001269
     22        1           0.000015946    0.000001272    0.000005966
     23        1           0.000022845    0.000009338   -0.000014286
     24        6          -0.000038612    0.000055701   -0.000090632
     25        1          -0.000023609   -0.000056582    0.000018334
     26        1          -0.000082054   -0.000052593    0.000018675
     27        1           0.000034428   -0.000014333    0.000005116
```

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000090632 RMS     0.000028120


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000270914 RMS     0.000042636
 Search for a local minimum.
 Step number  44 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   32   33   35   34
36
                                                     37   38   39   40
41
                                                     42   43   44
 DE= -2.68D-05 DEPred=-2.02D-05 R= 1.33D+00
 SS=  1.41D+00  RLast= 2.00D-01 DXNew= 3.3636D-01 6.0000D-01
 Trust test= 1.33D+00 RLast= 2.00D-01 DXMaxT set to 3.36D-01
     Eigenvalues ---    0.00008   0.00186   0.00988   0.01520
0.01657
     Eigenvalues ---    0.01775   0.01809   0.01824   0.01856
0.01927
     Eigenvalues ---    0.01973   0.01979   0.01995   0.02064
0.02090
     Eigenvalues ---    0.02106   0.02137   0.02145   0.02222
0.02227
     Eigenvalues ---    0.02309   0.02341   0.05850   0.06341
0.08386
     Eigenvalues ---    0.11386   0.12833   0.15511   0.15755
0.15980
     Eigenvalues ---    0.15999   0.16002   0.16002   0.16018
0.16044
     Eigenvalues ---    0.16420   0.17341   0.21328   0.22012
0.22562
     Eigenvalues ---    0.22714   0.22928   0.24062   0.24355
0.24578
     Eigenvalues ---    0.25184   0.27486   0.31514   0.32568
0.33097
     Eigenvalues ---    0.33591   0.33631   0.33642   0.33682
0.33684
     Eigenvalues ---    0.33960   0.34157   0.34710   0.36357
0.37321
     Eigenvalues ---    0.37582   0.38016   0.38364   0.39649
0.40327
     Eigenvalues ---    0.40502   0.40971   0.43561   0.44748
0.46203
     Eigenvalues ---    0.49070   0.49829   0.51100   0.51288
0.54664
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   8.12D-05 Eigenvector:
                          D45       D42       D44       D41       D46
   1                    0.40813   0.40002   0.38310   0.37499
0.36047
                          D43       D27       D28       D38       D40
   1                    0.35237  -0.11606  -0.10811   0.10696
0.09880
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    44   43   42   41
40
 RFO step:  Lambda=-6.77385873D-07.
 DIIS coeffs:      0.47344      0.12667      0.49923     -0.02123
-0.07811
 Iteration  1 RMS(Cart)=  0.00790267 RMS(Int)=  0.00010489
 Iteration  2 RMS(Cart)=  0.00010900 RMS(Int)=  0.00000074
 Iteration  3 RMS(Cart)=  0.00000002 RMS(Int)=  0.00000074
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59084  -0.00001   0.00010   0.00031   0.00041
2.59125
    R2        2.69163   0.00001  -0.00014  -0.00043  -0.00056
2.69107
```

This journal is © The Royal Society of Chemistry 2014

R3	2.05397	0.00001	0.00009	0.00005	0.00014
2.05411					
R4	2.70410	-0.00001	-0.00004	-0.00017	-0.00022
2.70388					
R5	2.05589	0.00001	0.00003	0.00008	0.00011
2.05599					
R6	2.73061	-0.00007	-0.00024	0.00030	0.00006
2.73067					
R7	2.64295	0.00000	-0.00014	-0.00027	-0.00041
2.64255					
R8	2.71046	-0.00006	-0.00020	-0.00022	-0.00042
2.71004					
R9	2.68006	-0.00010	-0.00025	-0.00027	-0.00051
2.67955					
R10	2.59571	0.00001	-0.00002	0.00013	0.00011
2.59582					
R11	2.04941	0.00005	0.00011	-0.00003	0.00008
2.04949					
R12	2.05439	0.00001	0.00015	0.00015	0.00029
2.05469					
R13	2.64087	0.00002	-0.00006	-0.00019	-0.00025
2.64062					
R14	2.05699	0.00001	0.00006	0.00008	0.00014
2.05713					
R15	2.67851	0.00009	-0.00005	0.00081	0.00075
2.67927					
R16	2.86178	0.00000	0.00010	0.00142	0.00153
2.86330					
R17	2.74075	0.00004	0.00012	0.00020	0.00031
2.74106					
R18	2.71458	0.00005	-0.00014	0.00042	0.00028
2.71486					
R19	2.70620	0.00000	-0.00001	-0.00022	-0.00023
2.70597					
R20	2.05585	0.00001	0.00003	0.00009	0.00012
2.05596					
R21	2.58820	-0.00006	0.00003	0.00019	0.00022
2.58843					
R22	2.69238	0.00000	-0.00017	-0.00058	-0.00075
2.69163					
R23	2.05388	0.00002	0.00009	0.00007	0.00016
2.05404					
R24	2.59348	-0.00002	-0.00009	0.00019	0.00010
2.59358					
R25	2.05435	0.00001	0.00015	0.00016	0.00030
2.05466					
R26	2.04772	0.00000	0.00005	-0.00038	-0.00034
2.04738					
R27	2.07510	0.00002	-0.00007	0.00000	-0.00007
2.07503					
R28	2.05901	-0.00009	-0.00025	0.00027	0.00002
2.05903					

This journal is © The Royal Society of Chemistry 2014

R29	2.07313	-0.00003	0.00038	-0.00053	-0.00015
2.07298					
A1	2.09061	0.00000	0.00008	-0.00004	0.00004
2.09065					
A2	2.10168	0.00001	0.00013	0.00073	0.00086
2.10254					
A3	2.09090	-0.00001	-0.00022	-0.00069	-0.00091
2.08999					
A4	2.11527	-0.00001	-0.00005	0.00012	0.00007
2.11534					
A5	2.10416	0.00001	0.00006	0.00041	0.00047
2.10463					
A6	2.06375	0.00000	0.00000	-0.00053	-0.00054
2.06322					
A7	2.08415	-0.00001	-0.00011	-0.00015	-0.00026
2.08389					
A8	2.11644	0.00003	0.00033	-0.00011	0.00022
2.11667					
A9	2.08259	-0.00002	-0.00022	0.00025	0.00004
2.08263					
A10	2.04768	0.00005	0.00022	-0.00006	0.00016
2.04784					
A11	2.09865	0.00006	0.00029	-0.00006	0.00024
2.09888					
A12	2.13686	-0.00011	-0.00051	0.00011	-0.00040
2.13646					
A13	2.12241	-0.00002	-0.00006	0.00015	0.00010
2.12250					
A14	2.08531	-0.00003	-0.00002	-0.00030	-0.00032
2.08499					
A15	2.07546	0.00004	0.00008	0.00014	0.00022
2.07568					
A16	2.10625	-0.00001	-0.00008	-0.00004	-0.00012
2.10614					
A17	2.08622	-0.00001	-0.00011	-0.00062	-0.00074
2.08549					
A18	2.09071	0.00002	0.00019	0.00066	0.00085
2.09156					
A19	2.11919	0.00000	0.00002	0.00003	0.00005
2.11923					
A20	2.08264	0.00000	0.00002	-0.00010	-0.00007
2.08256					
A21	2.08136	0.00001	-0.00004	0.00007	0.00003
2.08139					
A22	2.08822	0.00001	0.00007	-0.00023	-0.00017
2.08806					
A23	2.06855	-0.00027	-0.00147	0.00053	-0.00094
2.06761					
A24	2.12640	0.00026	0.00141	-0.00029	0.00111
2.12751					
A25	2.08750	-0.00007	-0.00033	0.00009	-0.00025
2.08726					

```
   A26        2.15678   0.00013   0.00051   0.00008   0.00059
2.15738
   A27        2.03890  -0.00006  -0.00018  -0.00017  -0.00035
2.03855
   A28        2.09018   0.00002   0.00019  -0.00009   0.00010
2.09028
   A29        2.10666  -0.00005  -0.00023   0.00021  -0.00002
2.10665
   A30        2.08634   0.00003   0.00004  -0.00012  -0.00008
2.08626
   A31        2.06120  -0.00002  -0.00010  -0.00055  -0.00065
2.06055
   A32        2.11762   0.00001   0.00003   0.00017   0.00020
2.11781
   A33        2.10437   0.00001   0.00007   0.00038   0.00045
2.10482
   A34        2.08784  -0.00001  -0.00009   0.00013   0.00004
2.08787
   A35        2.10329   0.00001   0.00023   0.00068   0.00091
2.10420
   A36        2.09206  -0.00001  -0.00014  -0.00080  -0.00095
2.09112
   A37        2.10854   0.00002   0.00004  -0.00013  -0.00009
2.10846
   A38        2.08625  -0.00002  -0.00009  -0.00074  -0.00083
2.08542
   A39        2.08839   0.00001   0.00005   0.00087   0.00092
2.08931
   A40        2.12712   0.00001   0.00016   0.00012   0.00028
2.12740
   A41        2.09091   0.00002   0.00029  -0.00049  -0.00021
2.09070
   A42        2.06515  -0.00003  -0.00045   0.00037  -0.00008
2.06507
   A43        1.94242  -0.00008  -0.00061   0.00036  -0.00025
1.94217
   A44        1.97299   0.00008   0.00131  -0.00068   0.00063
1.97361
   A45        1.93997  -0.00004  -0.00049   0.00051   0.00002
1.93999
   A46        1.86961   0.00001   0.00016  -0.00032  -0.00016
1.86945
   A47        1.86875   0.00003  -0.00006   0.00024   0.00019
1.86894
   A48        1.86473  -0.00001  -0.00035  -0.00011  -0.00046
1.86427
    D1       -0.00027   0.00000  -0.00011   0.00080   0.00069
0.00042
    D2        3.14039  -0.00001   0.00034  -0.00029   0.00005
3.14045
    D3       -3.14117   0.00001  -0.00012   0.00120   0.00109  -
3.14008
```

This journal is © The Royal Society of Chemistry 2014

D4	-0.00050	0.00000	0.00034	0.00011	0.00045	-0.00005
D5	0.00162	0.00001	-0.00043	0.00145	0.00101	0.00264
D6	-3.13958	0.00001	-0.00094	0.00128	0.00034	-3.13924
D7	-3.14067	0.00000	-0.00043	0.00105	0.00062	-3.14005
D8	0.00131	0.00000	-0.00093	0.00088	-0.00005	0.00126
D9	-0.00226	-0.00001	0.00084	-0.00237	-0.00153	-0.00379
D10	3.13878	-0.00001	0.00117	-0.00191	-0.00074	3.13804
D11	3.14024	-0.00001	0.00039	-0.00130	-0.00091	3.13933
D12	-0.00191	-0.00001	0.00072	-0.00085	-0.00012	-0.00203
D13	0.00338	0.00001	-0.00100	0.00170	0.00070	0.00408
D14	-3.13962	0.00000	-0.00056	0.00153	0.00097	-3.13866
D15	-3.13767	0.00001	-0.00133	0.00125	-0.00008	-3.13775
D16	0.00251	0.00000	-0.00089	0.00108	0.00019	0.00270
D17	-3.13770	0.00001	-0.00101	0.00012	-0.00089	-3.13859
D18	0.00144	0.00001	-0.00125	0.00159	0.00034	0.00178
D19	0.00334	0.00001	-0.00067	0.00058	-0.00010	0.00324
D20	-3.14070	0.00001	-0.00092	0.00205	0.00112	-3.13958
D21	-0.00212	0.00000	0.00048	0.00049	0.00097	-0.00114
D22	3.13670	-0.00001	0.00117	-0.00194	-0.00077	3.13593
D23	3.14092	0.00001	0.00003	0.00067	0.00070	-3.14157
D24	-0.00344	0.00000	0.00072	-0.00176	-0.00105	-0.00449
D25	-0.00886	-0.00001	0.00236	-0.00208	0.00029	-0.00858
D26	3.13650	-0.00002	0.00157	-0.00418	-0.00261	3.13389
D27	3.13124	-0.00003	0.00283	-0.00226	0.00057	3.13182
D28	-0.00658	-0.00003	0.00204	-0.00436	-0.00232	-0.00890
D29	-0.00037	-0.00001	0.00024	-0.00210	-0.00186	-0.00223

This journal is © The Royal Society of Chemistry 2014

D30	3.14084	-0.00001	0.00074	-0.00192	-0.00119	3.13965
D31	-3.13920	0.00000	-0.00045	0.00032	-0.00012	-3.13933
D32	0.00200	0.00000	0.00006	0.00049	0.00055	0.00255
D33	-0.00275	-0.00001	0.00073	-0.00120	-0.00046	-0.00321
D34	3.13764	-0.00001	0.00103	-0.00011	0.00092	3.13855
D35	3.14129	-0.00001	0.00098	-0.00267	-0.00168	3.13961
D36	-0.00151	0.00000	0.00128	-0.00158	-0.00030	-0.00181
D37	0.00941	0.00001	-0.00229	0.00145	-0.00084	0.00857
D38	-3.12955	0.00000	-0.00253	0.00040	-0.00213	-3.13168
D39	-3.13608	0.00001	-0.00148	0.00363	0.00215	-3.13394
D40	0.00814	0.00000	-0.00171	0.00258	0.00087	0.00901
D41	1.11402	-0.00004	-0.01621	-0.01078	-0.02699	1.08703
D42	-3.06419	-0.00002	-0.01553	-0.01141	-0.02694	-3.09113
D43	-0.96728	0.00000	-0.01543	-0.01166	-0.02708	-0.99436
D44	-2.02371	-0.00004	-0.01702	-0.01293	-0.02995	-2.05366
D45	0.08126	-0.00002	-0.01634	-0.01356	-0.02990	0.05136
D46	2.17817	0.00000	-0.01623	-0.01381	-0.03004	2.14813
D47	-0.00370	0.00000	0.00077	0.00017	0.00094	-0.00276
D48	3.13909	-0.00001	0.00047	-0.00090	-0.00042	3.13866
D49	3.13544	0.00001	0.00098	0.00115	0.00214	3.13757
D50	-0.00496	0.00000	0.00069	0.00008	0.00077	-0.00419
D51	-3.14068	0.00000	0.00004	-0.00099	-0.00095	3.14156
D52	0.00475	0.00000	-0.00045	0.00080	0.00035	0.00510
D53	0.00348	-0.00001	-0.00019	-0.00201	-0.00220	0.00128
D54	-3.13428	-0.00001	-0.00068	-0.00022	-0.00090	-3.13517
D55	0.00298	0.00000	-0.00063	-0.00054	-0.00116	0.00182

```
   D56       -3.13731   0.00000  -0.00103   0.00044  -0.00059  -
3.13790
   D57       -3.13981   0.00000  -0.00033   0.00054   0.00021  -
3.13960
   D58        0.00308   0.00000  -0.00073   0.00152   0.00079
0.00387
   D59        0.00056   0.00000   0.00024  -0.00124  -0.00100  -
0.00044
   D60        3.14092   0.00000   0.00012  -0.00108  -0.00096
3.13997
   D61       -3.13971   0.00000  -0.00017  -0.00024  -0.00041  -
3.14011
   D62        0.00066   0.00000  -0.00029  -0.00008  -0.00037
0.00030
   D63       -0.00217   0.00000   0.00028  -0.00071  -0.00042  -
0.00259
   D64        3.13858   0.00000   0.00074  -0.00035   0.00039
3.13897
   D65        3.14064   0.00000   0.00040  -0.00086  -0.00046
3.14017
   D66       -0.00180   0.00000   0.00086  -0.00051   0.00035  -
0.00145
   D67        0.00005   0.00001  -0.00030   0.00238   0.00207
0.00212
   D68        3.13786   0.00001   0.00018   0.00061   0.00079
3.13865
   D69       -3.14070   0.00001  -0.00076   0.00202   0.00126  -
3.13944
   D70       -0.00289   0.00001  -0.00028   0.00025  -0.00002  -
0.00292
         Item               Value     Threshold  Converged?
 Maximum Force            0.000271     0.000450     YES
 RMS     Force            0.000043     0.000300     YES
 Maximum Displacement     0.049970     0.001800     NO
 RMS     Displacement     0.007903     0.001200     NO
 Predicted change in Energy=-3.767440D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793449   -5.418119    0.016765
      2          6           0       -3.422515   -5.391657    0.006390
      3          6           0       -2.705127   -4.153712   -0.004689
      4          6           0       -3.438742   -2.908791   -0.009720
      5          6           0       -4.870587   -2.988206    0.002003
      6          6           0       -5.524599   -4.196091    0.016080
      7          6           0       -1.307064   -4.124844   -0.011032
```

8	6	0	-2.746305	-1.671491	-0.024286
9	6	0	-1.328533	-1.661441	-0.023336
10	6	0	-0.603346	-2.917644	-0.018271
11	6	0	0.828544	-2.906089	-0.020965
12	1	0	1.348066	-3.862002	-0.018963
13	6	0	1.531536	-1.730515	-0.023723
14	6	0	0.830275	-0.490755	-0.024480
15	6	0	-0.541829	-0.459347	-0.025536
16	1	0	-0.754470	-5.062744	-0.009155
17	1	0	-5.326352	-6.365465	0.026542
18	1	0	-2.850910	-6.317388	0.007850
19	1	0	-5.455478	-2.074899	0.004015
20	1	0	-6.611517	-4.222672	0.026560
21	1	0	2.618472	-1.736544	-0.024227
22	1	0	1.390590	0.441028	-0.024189
23	1	0	-1.033840	0.505918	-0.023275
24	6	0	-3.556026	-0.390888	-0.039348
25	1	0	-4.171219	-0.297755	0.865417
26	1	0	-2.938118	0.504472	-0.100456
27	1	0	-4.238886	-0.364373	-0.897454

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.371229	0.000000			
3	C	2.441368	1.430831	0.000000		
4	C	2.851782	2.482971	1.445006	0.000000	
5	C	2.431182	2.805978	2.459200	1.434094	0.000000
6	C	1.424055	2.418311	2.819867	2.451245	1.373651
7	C	3.718630	2.465816	1.398375	2.454147	3.740429
8	C	4.269627	3.781249	2.482640	1.417954	2.499401
9	C	5.110761	4.277868	2.847239	2.451336	3.782472
10	C	4.879607	3.750875	2.438346	2.835423	4.267873
11	C	6.157802	4.924460	3.747487	4.267302	5.699769
12	H	6.335691	5.009883	4.063701	4.880802	6.279777
13	C	7.321577	6.160153	4.880733	5.108051	6.524540
14	C	7.477091	6.488915	5.090846	4.906284	6.223969
15	C	6.532035	5.712010	4.281194	3.793696	5.013385
16	H	4.054666	2.688288	2.152074	3.441632	4.609366
17	H	1.086989	2.138529	3.429818	3.938652	3.407962
18	H	2.140612	1.087985	2.168618	3.458957	3.893916
19	H	3.408162	3.890222	3.447603	2.182381	1.084541
20	H	2.175905	3.396567	3.907123	3.434253	2.134325
21	H	8.276004	7.060758	5.846690	6.169620	7.592980
22	H	8.519015	7.562217	6.155235	5.877410	7.138814
23	H	7.016443	6.363021	4.950322	4.176599	5.189429
24	C	5.177588	5.002760	3.857988	2.520807	2.911329
25	H	5.227381	5.219801	4.216030	2.849544	2.910863
26	H	6.207502	5.916959	4.664990	3.450975	3.992961
27	H	5.165626	5.172715	4.184320	2.811115	2.844744

		6	7	8	9	10
6	C	0.000000				

This journal is © The Royal Society of Chemistry 2014

7	C	4.218223	0.000000			
8	C	3.754218	2.844386	0.000000		
9	C	4.902343	2.463527	1.417808	0.000000	
10	C	5.084716	1.397356	2.478953	1.450506	0.000000
11	C	6.482893	2.458920	3.782035	2.490409	1.431939
12	H	6.880869	2.668120	4.643516	3.465064	2.167907
13	C	7.474602	3.713573	4.278248	2.860903	2.442749
14	C	7.356330	4.216042	3.766439	2.455802	2.818705
15	C	6.228401	3.744552	2.515752	1.436641	2.459078
16	H	4.848284	1.088586	3.932968	3.449436	2.150436
17	H	2.178438	4.601790	5.356550	6.173564	5.847758
18	H	3.413001	2.681616	4.647186	4.898616	4.075596
19	H	2.122352	4.627292	2.739189	4.147694	4.924825
20	H	1.087294	5.305487	4.631519	5.871312	6.148433
21	H	8.506503	4.594996	5.365171	3.947719	3.431493
22	H	8.326123	5.303273	4.645066	3.437151	3.905956
23	H	6.502104	4.638831	2.770134	2.187302	3.450525
24	C	4.284614	4.359020	1.515196	2.564427	3.886291
25	H	4.213079	4.859852	2.170046	3.275727	4.513806
26	H	5.366447	4.909064	2.185729	2.699610	4.143525
27	H	4.143630	4.849997	2.167666	3.304031	4.528720

		11	12	13	14	15
11	C	0.000000				
12	H	1.087969	0.000000			
13	C	1.369736	2.139374	0.000000		
14	C	2.415337	3.410784	1.424350	0.000000	
15	C	2.804370	3.892276	2.432019	1.372465	0.000000
16	H	2.675301	2.421267	4.041012	4.838877	4.608335
17	H	7.060616	7.128622	8.277434	8.509929	7.601092
18	H	5.017587	4.864261	6.343991	6.892156	6.296794
19	H	6.338804	7.034378	6.995550	6.482362	5.172506
20	H	7.555803	7.967880	8.516024	8.325267	7.141879
21	H	2.138150	2.476193	1.086953	2.179366	3.408627
22	H	3.393979	4.303244	2.176113	1.087277	2.131882
23	H	3.887192	4.975160	3.403349	2.113831	1.083427
24	C	5.054803	6.008258	5.261001	4.387463	3.015006
25	H	5.708477	6.629366	5.946830	5.083710	3.740639
26	H	5.081928	6.119160	4.997886	3.898338	2.583943
27	H	5.736497	6.649751	5.993957	5.145333	3.799670

		16	17	18	19	20
16	H	0.000000				
17	H	4.753995	0.000000			
18	H	2.443252	2.475980	0.000000		
19	H	5.570177	4.292568	4.978202	0.000000	
20	H	5.917094	2.498642	4.304689	2.439234	0.000000
21	H	4.737147	9.195092	7.134374	8.081085	9.559084
22	H	5.907031	9.562857	7.979194	7.293787	9.262094
23	H	5.575683	8.102101	7.061176	5.119789	7.312491
24	C	5.447556	6.231690	5.968485	2.538836	4.901319
25	H	5.928252	6.233390	6.222107	2.355753	4.697202
26	H	5.980849	7.274327	6.823277	3.605713	5.987978
27	H	5.916496	6.168424	6.179356	2.284434	4.622731

This journal is © The Royal Society of Chemistry 2014

		21	22	23	24	25
21	H	0.000000				
22	H	2.499903	0.000000			
23	H	4.285792	2.425298	0.000000		
24	C	6.319450	5.016107	2.676928	0.000000	
25	H	6.997248	5.680750	3.358394	1.098060	0.000000
26	H	5.991966	4.329845	1.905843	1.089594	1.759834
27	H	7.047605	5.753456	3.434227	1.096971	1.765426

		26	27
26	H	0.000000	
27	H	1.755589	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.651976	-1.005327	0.004103
2	6	0	-2.452153	-1.669136	-0.003048
3	6	0	-1.211098	-0.957055	-0.003709
4	6	0	-1.222390	0.487906	-0.001487
5	6	0	-2.501462	1.136393	0.006500
6	6	0	-3.672625	0.418564	0.010514
7	6	0	0.013387	-1.632392	-0.006751
8	6	0	-0.003233	1.211945	-0.005695
9	6	0	1.228843	0.510411	-0.001534
10	6	0	1.227189	-0.940092	-0.003822
11	6	0	2.472259	-1.647377	-0.003263
12	1	0	2.443044	-2.734948	-0.006929
13	6	0	3.669565	-0.982107	0.003919
14	6	0	3.683666	0.442158	0.010451
15	6	0	2.511882	1.156696	0.006581
16	1	0	0.021821	-2.720940	-0.010339
17	1	0	-4.587789	-1.558314	0.005943
18	1	0	-2.421168	-2.756672	-0.006925
19	1	0	-2.550188	2.219815	0.013730
20	1	0	-4.626699	0.939994	0.018398
21	1	0	4.607265	-1.531818	0.005778
22	1	0	4.635353	0.967894	0.018627
23	1	0	2.569567	2.238556	0.014637
24	6	0	-0.062465	2.725963	-0.013416
25	1	0	-0.553213	3.110164	0.890625
26	1	0	0.921159	3.191637	-0.066769
27	1	0	-0.635472	3.095332	-0.872821

Rotational constants (GHZ): 1.3940520 0.4478255
0.3396635

This journal is © The Royal Society of Chemistry 2014

```
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9015336358 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
```

```
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860686547     A.U. after   10 cycles
             Convg  =    0.4872D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000227989   -0.000168702    0.000013465
      2        6          -0.000142730   -0.000126883    0.000076696
      3        6          -0.000247027    0.000082333   -0.000055074
      4        6           0.000039762   -0.000122354   -0.000007911
      5        6          -0.000182641    0.000026642    0.000130544
      6        6          -0.000111322    0.000140796   -0.000077510
      7        6           0.000121880   -0.000153574   -0.000029883
      8        6           0.000161244    0.000423773   -0.000032098
      9        6          -0.000142532    0.000072373   -0.000070020
     10        6          -0.000035564    0.000239696   -0.000075077
     11        6           0.000167556    0.000007919    0.000086141
     12        1           0.000039524    0.000048320   -0.000000173
     13        6           0.000103681   -0.000290835    0.000008925
     14        6          -0.000133782    0.000191475   -0.000073802
     15        6          -0.000023828   -0.000082597    0.000154125
     16        1          -0.000011713    0.000029606    0.000020958
     17        1           0.000113751   -0.000021790   -0.000017816
     18        1          -0.000061904   -0.000014413    0.000011212
     19        1          -0.000013597    0.000016665   -0.000063788
     20        1           0.000093364    0.000091041    0.000000298
     21        1          -0.000039266   -0.000115296   -0.000016621
     22        1          -0.000144820   -0.000030724   -0.000005127
     23        1          -0.000074469    0.000134931   -0.000051777
     24        6           0.000334717   -0.000133348    0.000129826
     25        1           0.000091020   -0.000021825   -0.000066228
     26        1           0.000008145   -0.000085352    0.000125612
     27        1          -0.000137441   -0.000137880   -0.000114897
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000423773 RMS     0.000121967
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000478978 RMS     0.000087003
 Search for a local minimum.
 Step number  45 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   35   34   36   37
38
                                                     39   40   41   42
43
                                                     44   45
 DE= -1.70D-07 DEPred=-3.77D-06 R= 4.51D-02
 Trust test= 4.51D-02 RLast= 7.05D-02 DXMaxT set to 1.68D-01
     Eigenvalues ---    0.00004   0.00851   0.01468   0.01537
0.01759
     Eigenvalues ---    0.01778   0.01814   0.01843   0.01915
0.01968
     Eigenvalues ---    0.01976   0.01996   0.02024   0.02066
0.02107
     Eigenvalues ---    0.02109   0.02146   0.02188   0.02214
0.02227
     Eigenvalues ---    0.02341   0.02349   0.05588   0.06413
0.09994
     Eigenvalues ---    0.11310   0.15347   0.15500   0.15734
0.15936
     Eigenvalues ---    0.15998   0.16000   0.16003   0.16004
0.16072
     Eigenvalues ---    0.16086   0.19366   0.21776   0.22072
0.22579
     Eigenvalues ---    0.22730   0.22781   0.23577   0.24526
0.24749
     Eigenvalues ---    0.25317   0.27733   0.29026   0.31735
0.32547
     Eigenvalues ---    0.33569   0.33600   0.33631   0.33682
0.33684
     Eigenvalues ---    0.33845   0.34069   0.34700   0.35496
0.37315
     Eigenvalues ---    0.37421   0.37853   0.38199   0.39619
0.40243
     Eigenvalues ---    0.40805   0.41266   0.43593   0.44547
0.46158
     Eigenvalues ---    0.48447   0.49813   0.50671   0.51520
0.52114
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvalue     1 is   4.48D-05 Eigenvector:
                          D45       D44       D42       D46       D41
   1                    0.42634   0.41126   0.40494   0.39043
0.38987
                          D43       D27       D38       D25       D37
   1                    0.36903  -0.07418   0.06888  -0.05909
0.05715
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    45   44   43   42
41
 RFO step:  Lambda=-2.66704506D-06.
 DIIS coeffs:      0.13112      1.06096     -0.23712      0.33031
-0.28526
 Iteration  1 RMS(Cart)=  0.01283069 RMS(Int)=  0.00020767
 Iteration  2 RMS(Cart)=  0.00021569 RMS(Int)=  0.00000213
 Iteration  3 RMS(Cart)=  0.00000006 RMS(Int)=  0.00000213
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                   (DIIS)     (GDIIS)  (Total)
    R1        2.59125  -0.00022  -0.00016  -0.00027  -0.00043
2.59082
    R2        2.69107   0.00027   0.00027   0.00044   0.00071
2.69178
    R3        2.05411  -0.00004  -0.00005  -0.00014  -0.00019
2.05392
    R4        2.70388   0.00007   0.00006   0.00008   0.00014
2.70402
```

This journal is © The Royal Society of Chemistry 2014

R5	2.05599	-0.00002	-0.00007	0.00000	-0.00008
2.05592					
R6	2.73067	-0.00004	-0.00025	-0.00034	-0.00060
2.73007					
R7	2.64255	0.00017	0.00015	0.00051	0.00067
2.64322					
R8	2.71004	0.00009	0.00026	0.00023	0.00049
2.71054					
R9	2.67955	0.00012	0.00027	0.00060	0.00087
2.68042					
R10	2.59582	-0.00004	-0.00022	0.00002	-0.00019
2.59563					
R11	2.04949	0.00002	-0.00003	-0.00007	-0.00010
2.04939					
R12	2.05469	-0.00010	-0.00009	-0.00022	-0.00032
2.05437					
R13	2.64062	0.00016	-0.00004	0.00008	0.00004
2.64066					
R14	2.05713	-0.00003	-0.00005	-0.00008	-0.00013
2.05700					
R15	2.67927	-0.00035	-0.00107	-0.00046	-0.00154
2.67773					
R16	2.86330	-0.00048	-0.00023	-0.00111	-0.00135
2.86196					
R17	2.74106	-0.00003	0.00009	0.00005	0.00013
2.74119					
R18	2.71486	-0.00015	-0.00033	0.00030	-0.00003
2.71483					
R19	2.70597	0.00007	0.00018	0.00027	0.00045
2.70642					
R20	2.05596	-0.00002	-0.00009	0.00000	-0.00009
2.05587					
R21	2.58843	-0.00018	-0.00008	-0.00038	-0.00046
2.58796					
R22	2.69163	0.00034	0.00046	0.00069	0.00115
2.69278					
R23	2.05404	-0.00004	-0.00007	-0.00015	-0.00022
2.05382					
R24	2.59358	-0.00008	-0.00032	-0.00013	-0.00045
2.59313					
R25	2.05466	-0.00010	-0.00010	-0.00023	-0.00033
2.05432					
R26	2.04738	0.00015	0.00028	0.00005	0.00033
2.04771					
R27	2.07503	-0.00011	-0.00046	-0.00030	-0.00075
2.07428					
R28	2.05903	-0.00007	-0.00052	-0.00008	-0.00059
2.05844					
R29	2.07298	0.00017	0.00092	0.00052	0.00143
2.07441					
A1	2.09065	0.00001	0.00022	-0.00019	0.00003
2.09068					

This journal is © The Royal Society of Chemistry 2014

A2	2.10254	-0.00012	-0.00116	-0.00005	-0.00120
2.10134					
A3	2.08999	0.00011	0.00094	0.00023	0.00118
2.09117					
A4	2.11534	-0.00003	-0.00003	-0.00007	-0.00010
2.11524					
A5	2.10463	-0.00005	-0.00105	0.00016	-0.00089
2.10374					
A6	2.06322	0.00008	0.00108	-0.00010	0.00099
2.06420					
A7	2.08389	0.00007	-0.00014	0.00036	0.00023
2.08411					
A8	2.11667	0.00001	0.00048	-0.00031	0.00017
2.11684					
A9	2.08263	-0.00008	-0.00034	-0.00005	-0.00040
2.08223					
A10	2.04784	0.00001	0.00023	-0.00015	0.00007
2.04791					
A11	2.09888	-0.00002	0.00007	0.00005	0.00012
2.09900					
A12	2.13646	0.00001	-0.00029	0.00010	-0.00019
2.13627					
A13	2.12250	-0.00008	-0.00006	-0.00013	-0.00019
2.12232					
A14	2.08499	0.00004	0.00003	0.00001	0.00005
2.08504					
A15	2.07568	0.00004	0.00003	0.00012	0.00015
2.07583					
A16	2.10614	0.00003	-0.00021	0.00018	-0.00003
2.10611					
A17	2.08549	0.00008	0.00076	0.00011	0.00086
2.08635					
A18	2.09156	-0.00010	-0.00055	-0.00028	-0.00083
2.09072					
A19	2.11923	-0.00002	0.00002	-0.00009	-0.00007
2.11916					
A20	2.08256	0.00002	0.00010	0.00006	0.00016
2.08272					
A21	2.08139	0.00001	-0.00012	0.00003	-0.00009
2.08130					
A22	2.08806	0.00011	0.00039	-0.00006	0.00032
2.08838					
A23	2.06761	-0.00003	-0.00138	-0.00019	-0.00157
2.06604					
A24	2.12751	-0.00009	0.00100	0.00025	0.00125
2.12877					
A25	2.08726	0.00001	-0.00030	0.00015	-0.00016
2.08710					
A26	2.15738	-0.00011	0.00020	-0.00001	0.00019
2.15757					
A27	2.03855	0.00009	0.00010	-0.00014	-0.00004
2.03852					

This journal is © The Royal Society of Chemistry 2014

```
   A28        2.09028  -0.00001   0.00022   0.00000   0.00022
2.09049
   A29        2.10665  -0.00003  -0.00012  -0.00022  -0.00033
2.10631
   A30        2.08626   0.00003  -0.00010   0.00022   0.00011
2.08638
   A31        2.06055   0.00009   0.00107  -0.00022   0.00086
2.06140
   A32        2.11781  -0.00006  -0.00002   0.00000  -0.00003
2.11779
   A33        2.10482  -0.00003  -0.00105   0.00022  -0.00083
2.10399
   A34        2.08787  -0.00002  -0.00003  -0.00017  -0.00020
2.08768
   A35        2.10420  -0.00011  -0.00107  -0.00005  -0.00112
2.10307
   A36        2.09112   0.00013   0.00110   0.00022   0.00132
2.09244
   A37        2.10846   0.00004  -0.00008   0.00019   0.00011
2.10857
   A38        2.08542   0.00009   0.00082   0.00014   0.00096
2.08638
   A39        2.08931  -0.00013  -0.00075  -0.00033  -0.00107
2.08824
   A40        2.12740  -0.00008   0.00014  -0.00009   0.00004
2.12744
   A41        2.09070   0.00004   0.00048  -0.00015   0.00033
2.09103
   A42        2.06507   0.00005  -0.00061   0.00025  -0.00036
2.06471
   A43        1.94217  -0.00004  -0.00168  -0.00069  -0.00237
1.93979
   A44        1.97361  -0.00003   0.00081   0.00049   0.00130
1.97491
   A45        1.93999  -0.00012  -0.00089   0.00043  -0.00046
1.93953
   A46        1.86945  -0.00001   0.00055  -0.00151  -0.00097
1.86848
   A47        1.86894   0.00005   0.00012  -0.00059  -0.00047
1.86846
   A48        1.86427   0.00016   0.00121   0.00185   0.00306
1.86733
    D1        0.00042  -0.00002  -0.00045   0.00005  -0.00040
0.00001
    D2        3.14045   0.00001   0.00095   0.00016   0.00111
3.14156
    D3       -3.14008  -0.00003  -0.00111  -0.00046  -0.00158
3.14153
    D4       -0.00005  -0.00001   0.00029  -0.00035  -0.00006  -
0.00011
    D5        0.00264  -0.00002  -0.00187  -0.00065  -0.00252
0.00011
```

This journal is © The Royal Society of Chemistry 2014

D6	-3.13924	-0.00001	-0.00217	0.00008	-0.00209	-3.14133
D7	-3.14005	-0.00001	-0.00121	-0.00014	-0.00135	-3.14140
D8	0.00126	0.00001	-0.00151	0.00059	-0.00092	0.00034
D9	-0.00379	0.00004	0.00299	0.00058	0.00357	-0.00022
D10	3.13804	0.00003	0.00317	0.00012	0.00329	3.14133
D11	3.13933	0.00002	0.00162	0.00047	0.00209	3.14142
D12	-0.00203	0.00000	0.00180	0.00002	0.00181	-0.00022
D13	0.00408	-0.00002	-0.00317	-0.00061	-0.00378	0.00030
D14	-3.13866	-0.00002	-0.00177	-0.00058	-0.00235	-3.14101
D15	-3.13775	-0.00001	-0.00335	-0.00016	-0.00351	-3.14126
D16	0.00270	-0.00001	-0.00195	-0.00013	-0.00208	0.00062
D17	-3.13859	0.00000	-0.00219	-0.00045	-0.00263	-3.14122
D18	0.00178	0.00000	-0.00240	0.00087	-0.00152	0.00026
D19	0.00324	-0.00001	-0.00201	-0.00090	-0.00291	0.00033
D20	-3.13958	-0.00002	-0.00222	0.00042	-0.00180	-3.14138
D21	-0.00114	-0.00002	0.00094	0.00002	0.00097	-0.00018
D22	3.13593	0.00004	0.00373	0.00137	0.00510	3.14104
D23	-3.14157	-0.00002	-0.00049	0.00000	-0.00050	3.14112
D24	-0.00449	0.00004	0.00230	0.00135	0.00364	-0.00085
D25	-0.00858	0.00003	0.00536	0.00146	0.00682	-0.00176
D26	3.13389	0.00005	0.00491	0.00159	0.00650	3.14040
D27	3.13182	0.00003	0.00684	0.00148	0.00832	3.14014
D28	-0.00890	0.00004	0.00638	0.00162	0.00800	-0.00090
D29	-0.00223	0.00004	0.00159	0.00061	0.00220	-0.00003
D30	3.13965	0.00002	0.00189	-0.00012	0.00176	3.14141
D31	-3.13933	-0.00001	-0.00118	-0.00073	-0.00191	-3.14124

This journal is © The Royal Society of Chemistry 2014

D32	0.00255	-0.00003	-0.00088	-0.00147	-0.00235	0.00020
D33	-0.00321	0.00001	0.00247	0.00060	0.00307	-0.00014
D34	3.13855	-0.00001	0.00204	0.00037	0.00242	3.14097
D35	3.13961	0.00002	0.00268	-0.00072	0.00196	3.14157
D36	-0.00181	0.00000	0.00225	-0.00095	0.00130	-0.00051
D37	0.00857	-0.00002	-0.00488	-0.00175	-0.00663	0.00194
D38	-3.13168	-0.00001	-0.00468	-0.00241	-0.00709	-3.13877
D39	-3.13394	-0.00004	-0.00441	-0.00189	-0.00630	-3.14024
D40	0.00901	-0.00003	-0.00421	-0.00255	-0.00676	0.00225
D41	1.08703	0.00000	-0.01299	-0.02665	-0.03964	1.04739
D42	-3.09113	-0.00006	-0.01294	-0.02876	-0.04170	-3.13283
D43	-0.99436	0.00004	-0.01145	-0.02573	-0.03717	-1.03154
D44	-2.05366	0.00001	-0.01346	-0.02651	-0.03996	-2.09363
D45	0.05136	-0.00004	-0.01340	-0.02862	-0.04202	0.00934
D46	2.14813	0.00006	-0.01191	-0.02559	-0.03750	2.11063
D47	-0.00276	0.00000	0.00101	0.00074	0.00175	-0.00101
D48	3.13866	0.00002	0.00144	0.00096	0.00240	3.14107
D49	3.13757	-0.00001	0.00083	0.00135	0.00218	3.13976
D50	-0.00419	0.00001	0.00125	0.00158	0.00283	-0.00135
D51	3.14156	0.00001	0.00048	-0.00028	0.00020	-3.14143
D52	0.00510	-0.00004	-0.00180	-0.00225	-0.00406	0.00105
D53	0.00128	0.00003	0.00067	-0.00092	-0.00025	0.00103
D54	-3.13517	-0.00002	-0.00161	-0.00290	-0.00451	-3.13968
D55	0.00182	0.00001	-0.00031	-0.00046	-0.00077	0.00105
D56	-3.13790	-0.00002	-0.00163	-0.00075	-0.00238	-3.14028
D57	-3.13960	-0.00001	-0.00073	-0.00069	-0.00142	-3.14102

```
   D58        0.00387  -0.00004  -0.00206  -0.00098  -0.00304
0.00083
   D59       -0.00044   0.00002   0.00090  -0.00035   0.00055
0.00010
   D60        3.13997   0.00003   0.00087   0.00054   0.00140
3.14137
   D61       -3.14011   0.00000  -0.00046  -0.00065  -0.00111  -
3.14123
   D62        0.00030   0.00000  -0.00049   0.00024  -0.00026
0.00004
   D63       -0.00259   0.00002   0.00108   0.00105   0.00213  -
0.00046
   D64        3.13897   0.00000   0.00130   0.00051   0.00181
3.14078
   D65        3.14017   0.00001   0.00111   0.00017   0.00128
3.14146
   D66       -0.00145   0.00000   0.00133  -0.00037   0.00096  -
0.00049
   D67        0.00212  -0.00004  -0.00187  -0.00039  -0.00226  -
0.00014
   D68        3.13865   0.00001   0.00038   0.00156   0.00194
3.14059
   D69       -3.13944  -0.00003  -0.00209   0.00016  -0.00193  -
3.14137
   D70       -0.00292   0.00002   0.00016   0.00211   0.00227  -
0.00065
         Item               Value     Threshold  Converged?
 Maximum Force            0.000479     0.000450     NO
 RMS     Force            0.000087     0.000300     YES
 Maximum Displacement     0.101073     0.001800     NO
 RMS     Displacement     0.012828     0.001200     NO
 Predicted change in Energy=-7.065517D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793618   -5.417496    0.016222
      2          6           0       -3.422872   -5.391351    0.011433
      3          6           0       -2.705260   -4.153454   -0.000355
      4          6           0       -3.438252   -2.908546   -0.007615
      5          6           0       -4.870427   -2.987378   -0.002108
      6          6           0       -5.524719   -4.195022    0.009388
      7          6           0       -1.306837   -4.124541   -0.004947
      8          6           0       -2.745252   -1.671007   -0.020037
      9          6           0       -1.328297   -1.660938   -0.023140
     10          6           0       -0.603227   -2.917280   -0.016013
     11          6           0        0.828899   -2.906071   -0.019812
```

12	1	0	1.348994	-3.861606	-0.014856
13	6	0	1.532000	-1.730883	-0.029099
14	6	0	0.830448	-0.490601	-0.035014
15	6	0	-0.541411	-0.459015	-0.032065
16	1	0	-0.754098	-5.062264	0.000315
17	1	0	-5.325578	-6.365266	0.025129
18	1	0	-2.852326	-6.317673	0.016586
19	1	0	-5.454969	-2.073918	-0.006749
20	1	0	-6.611539	-4.220455	0.013472
21	1	0	2.618806	-1.738367	-0.031670
22	1	0	1.389782	0.441542	-0.041613
23	1	0	-1.033032	0.506641	-0.035838
24	6	0	-3.556248	-0.391996	-0.028880
25	1	0	-4.198096	-0.324047	0.858968
26	1	0	-2.939826	0.505904	-0.046971
27	1	0	-4.214474	-0.346928	-0.906215

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.371004	0.000000			
3	C	2.441171	1.430907	0.000000		
4	C	2.851740	2.482926	1.444689	0.000000	
5	C	2.431401	2.806187	2.459204	1.434354	0.000000
6	C	1.424429	2.418463	2.819782	2.451256	1.373548
7	C	3.718847	2.466309	1.398729	2.453891	3.740631
8	C	4.270047	3.781682	2.482847	1.418417	2.499905
9	C	5.110942	4.278367	2.847663	2.451260	3.782403
10	C	4.879702	3.751290	2.438629	2.835050	4.267798
11	C	6.158024	4.924952	3.747882	4.267169	5.699934
12	H	6.336675	5.011140	4.064771	4.881199	6.280576
13	C	7.321654	6.160473	4.880989	5.107911	6.524614
14	C	7.477102	6.489241	5.091064	4.906018	6.223742
15	C	6.532238	5.712500	4.281604	3.793743	5.013372
16	H	4.055141	2.689011	2.152434	3.441403	4.609699
17	H	1.086889	2.137519	3.429115	3.938526	3.408524
18	H	2.139845	1.087944	2.169276	3.459197	3.894091
19	H	3.408435	3.890387	3.447523	2.182602	1.084491
20	H	2.176638	3.396851	3.906879	3.433847	2.133587
21	H	8.275404	7.060313	5.846307	6.169104	7.592727
22	H	8.518574	7.562215	6.155084	5.876577	7.137875
23	H	7.017130	6.363951	4.951170	4.177245	5.189885
24	C	5.175787	5.001296	3.856625	2.519404	2.909259
25	H	5.196931	5.195850	4.198971	2.829835	2.878682
26	H	6.207029	5.917293	4.665492	3.450861	3.991523
27	H	5.186228	5.187958	4.193799	2.823453	2.866995

		6	7	8	9	10
6	C	0.000000				
7	C	4.218495	0.000000			
8	C	3.754591	2.844134	0.000000		
9	C	4.902305	2.463764	1.416995	0.000000	
10	C	5.084717	1.397379	2.478202	1.450576	0.000000

This journal is © The Royal Society of Chemistry 2014

11	C	6.483109	2.458914	3.781526	2.490755	1.432175
12	H	6.881837	2.668833	4.643447	3.465673	2.168622
13	C	7.474674	3.713378	4.277681	2.861158	2.442725
14	C	7.356144	4.215972	3.765530	2.455608	2.818609
15	C	6.228389	3.744689	2.515151	1.436624	2.459095
16	H	4.848816	1.088519	3.932650	3.449532	2.150346
17	H	2.179418	4.601308	5.356883	6.173434	5.847298
18	H	3.412826	2.683063	4.648044	4.899941	4.077030
19	H	2.122312	4.627317	2.739540	4.147318	4.924504
20	H	1.087126	5.305602	4.631305	5.870700	6.148085
21	H	8.506106	4.594041	5.364493	3.947871	3.430973
22	H	8.325302	5.303038	4.643472	3.436381	3.905691
23	H	6.502532	4.639371	2.770216	2.187633	3.450849
24	C	4.282446	4.358018	1.514484	2.563984	3.885557
25	H	4.179254	4.852782	2.167420	3.286509	4.518134
26	H	5.365031	4.910137	2.185755	2.700518	4.144736
27	H	4.166881	4.851495	2.167281	3.291879	4.521092

		11	12	13	14	15
11	C	0.000000				
12	H	1.087920	0.000000			
13	C	1.369491	2.138615	0.000000		
14	C	2.415519	3.410714	1.424960	0.000000	
15	C	2.804637	3.892500	2.432425	1.372226	0.000000
16	H	2.674968	2.421736	4.040447	4.838609	4.608274
17	H	7.060144	7.128803	8.276885	8.509523	7.601009
18	H	5.019140	4.866656	6.345316	6.893494	6.298140
19	H	6.338742	7.034899	6.995421	6.481833	5.172195
20	H	7.555716	7.968668	8.515693	8.324503	7.141216
21	H	2.137157	2.474035	1.086834	2.180632	3.409357
22	H	3.394345	4.303424	2.177111	1.087100	2.130868
23	H	3.887627	4.975547	3.403814	2.113540	1.083603
24	C	5.054718	6.008310	5.261453	4.387809	3.015584
25	H	5.719247	6.636875	5.966729	5.110108	3.766099
26	H	5.083857	6.121286	5.000076	3.899760	2.585282
27	H	5.724556	6.640757	5.975503	5.121609	3.777313

		16	17	18	19	20
16	H	0.000000				
17	H	4.753616	0.000000			
18	H	2.445174	2.473725	0.000000		
19	H	5.570319	4.293417	4.978328	0.000000	
20	H	5.917638	2.500809	4.304651	2.438378	0.000000
21	H	4.735588	9.193729	7.134819	8.080783	9.558351
22	H	5.906764	9.562068	7.980341	7.292418	9.260583
23	H	5.576003	8.102640	7.062849	5.119927	7.312155
24	C	5.446495	6.230040	5.967514	2.536630	4.898336
25	H	5.920230	6.201841	6.200344	2.321905	4.660640
26	H	5.981985	7.273926	6.824434	3.603199	5.985282
27	H	5.918648	6.190504	6.193287	2.308757	4.647145

		21	22	23	24	25
21	H	0.000000				
22	H	2.502519	0.000000			
23	H	4.286723	2.423695	0.000000		

```
   24  C    6.320128   5.015791   2.678473   0.000000
   25  H    7.018810   5.711528   3.392396   1.097661   0.000000
   26  H    5.994612   4.330089   1.906826   1.089279   1.758633
   27  H    7.028133   5.725112   3.407009   1.097729   1.765407
                 26         27
   26  H    0.000000
   27  H    1.757940   0.000000
 Stoichiometry    C15H12
 Framework group  C1[X(C15H12)]
 Deg. of freedom    75
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.651803   -1.005595    0.000964
      2          6           0       -2.452188   -1.669352   -0.000015
      3          6           0       -1.211113   -0.957153   -0.000452
      4          6           0       -1.222173    0.487494   -0.000127
      5          6           0       -2.501346    1.136404    0.001006
      6          6           0       -3.672462    0.418684    0.001548
      7          6           0        0.013844   -1.632375   -0.001139
      8          6           0       -0.002577    1.211711   -0.001265
      9          6           0        1.228976    0.510890   -0.000559
     10          6           0        1.227454   -0.939685   -0.001125
     11          6           0        2.472714   -1.647113   -0.001067
     12          1           0        2.444406   -2.734664   -0.002044
     13          6           0        3.669813   -0.981939    0.000481
     14          6           0        3.683642    0.442952    0.002198
     15          6           0        2.511982    1.157247    0.001775
     16          1           0        0.022709   -2.720858   -0.001590
     17          1           0       -4.586888   -1.559620    0.001226
     18          1           0       -2.422199   -2.756883   -0.000440
     19          1           0       -2.549892    2.219807    0.001807
     20          1           0       -4.625955    0.940884    0.002576
     21          1           0        4.606802   -1.532631    0.000714
     22          1           0        4.634582    0.969731    0.004197
     23          1           0        2.569998    2.239293    0.004088
     24          6           0       -0.064070    2.724946   -0.002468
     25          1           0       -0.591041    3.100469    0.884180
     26          1           0        0.919209    3.193559   -0.012072
     27          1           0       -0.605895    3.098215   -0.881163
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3943584      0.4478233
0.3396759
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
```

```
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9259412807 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
```

```
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860689534     A.U. after   11 cycles
             Convg  =    0.3948D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000014878    0.000061436   -0.000014238
      2        6          -0.000008391   -0.000011526    0.000004500
      3        6           0.000068564   -0.000017835    0.000020501
      4        6          -0.000043990    0.000056266   -0.000063982
      5        6           0.000138335    0.000028239    0.000002847
      6        6           0.000023997   -0.000091422    0.000017393
      7        6          -0.000055620   -0.000040258   -0.000034796
      8        6          -0.000308273   -0.000074556    0.000030509
      9        6           0.000243365   -0.000039084    0.000038195
     10        6           0.000059927    0.000045030    0.000023120
     11        6          -0.000006905    0.000021431   -0.000001588
     12        1          -0.000044190   -0.000032034    0.000007299
     13        6          -0.000094051    0.000065585   -0.000011752
     14        6           0.000110148   -0.000100342    0.000015166
     15        6          -0.000115151    0.000024735   -0.000021454
     16        1          -0.000006764   -0.000011565   -0.000000758
     17        1          -0.000056520   -0.000003211    0.000004186
     18        1           0.000050174    0.000024999    0.000001839
     19        1          -0.000046064    0.000005517   -0.000002319
     20        1          -0.000018195   -0.000024701   -0.000001489
     21        1           0.000036532    0.000051310   -0.000003844
     22        1           0.000036333    0.000000674    0.000000990
     23        1          -0.000068187    0.000015333   -0.000022093
     24        6          -0.000105313   -0.000182757   -0.000100898
     25        1           0.000035918    0.000103705   -0.000003818
     26        1           0.000095815    0.000065085    0.000023145
     27        1           0.000093383    0.000059945    0.000093339
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000308273 RMS     0.000070244


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
```

This journal is © The Royal Society of Chemistry 2014

```
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000338091 RMS     0.000056513
 Search for a local minimum.
 Step number  46 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   37   38   39   40
41
                                                     42   43   44   45
46
 DE= -2.99D-06 DEPred=-7.07D-06 R= 4.23D-01
 Trust test= 4.23D-01 RLast= 1.01D-01 DXMaxT set to 1.68D-01
     Eigenvalues ---    0.00018   0.00698   0.01253   0.01578
0.01724
     Eigenvalues ---    0.01770   0.01798   0.01816   0.01895
0.01926
     Eigenvalues ---    0.01973   0.01982   0.02008   0.02063
0.02103
     Eigenvalues ---    0.02111   0.02145   0.02197   0.02209
0.02226
     Eigenvalues ---    0.02339   0.02361   0.05146   0.06653
0.10607
     Eigenvalues ---    0.11629   0.15466   0.15550   0.15628
0.15997
     Eigenvalues ---    0.16001   0.16002   0.16005   0.16027
0.16051
     Eigenvalues ---    0.16508   0.19216   0.20803   0.22002
0.22548
     Eigenvalues ---    0.22715   0.23091   0.23515   0.24457
0.24675
     Eigenvalues ---    0.25299   0.28401   0.29155   0.31615
0.32618
     Eigenvalues ---    0.33567   0.33597   0.33631   0.33682
0.33684
     Eigenvalues ---    0.33863   0.34029   0.34738   0.35474
0.37263
     Eigenvalues ---    0.37493   0.37846   0.38165   0.39712
0.40273
     Eigenvalues ---    0.40888   0.41010   0.43135   0.44624
0.45784
     Eigenvalues ---    0.49156   0.49821   0.50943   0.51668
0.53016
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    46   45   44   43
42
 RFO step:  Lambda=-8.52597143D-07.
 DIIS coeffs:      0.78185      0.17395     -0.65282      0.49345
0.20358
 Iteration  1 RMS(Cart)=  0.01180435 RMS(Int)=  0.00021026
 Iteration  2 RMS(Cart)=  0.00021778 RMS(Int)=  0.00000248
 Iteration  3 RMS(Cart)=  0.00000006 RMS(Int)=  0.00000248
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59082   0.00003   0.00003  -0.00007  -0.00004
2.59078
    R2        2.69178  -0.00007  -0.00018   0.00006  -0.00012
2.69166
    R3        2.05392   0.00003   0.00005   0.00006   0.00012
2.05404
    R4        2.70402  -0.00002   0.00003   0.00000   0.00003
2.70405
    R5        2.05592   0.00000   0.00001   0.00004   0.00005
2.05597
    R6        2.73007   0.00008   0.00046  -0.00009   0.00038
2.73045
    R7        2.64322  -0.00001  -0.00024   0.00008  -0.00017
2.64305
    R8        2.71054  -0.00005  -0.00004  -0.00006  -0.00010
2.71044
    R9        2.68042  -0.00003  -0.00030   0.00000  -0.00030
2.68012
   R10        2.59563   0.00007   0.00002   0.00005   0.00008
2.59571
```

This journal is © The Royal Society of Chemistry 2014

R11	2.04939	0.00003	-0.00001	0.00014	0.00013
2.04952					
R12	2.05437	0.00002	0.00008	-0.00001	0.00007
2.05444					
R13	2.64066	0.00003	0.00009	0.00012	0.00020
2.64087					
R14	2.05700	0.00001	0.00003	0.00002	0.00005
2.05706					
R15	2.67773	0.00011	0.00051	0.00013	0.00064
2.67837					
R16	2.86196	-0.00003	0.00014	-0.00024	-0.00009
2.86187					
R17	2.74119	-0.00008	-0.00037	-0.00007	-0.00043
2.74076					
R18	2.71483	-0.00005	-0.00018	0.00000	-0.00018
2.71465					
R19	2.70642	-0.00004	-0.00019	-0.00001	-0.00020
2.70622					
R20	2.05587	0.00001	0.00002	0.00003	0.00005
2.05593					
R21	2.58796	0.00005	0.00020	-0.00009	0.00011
2.58808					
R22	2.69278	-0.00009	-0.00035	0.00005	-0.00031
2.69248					
R23	2.05382	0.00004	0.00007	0.00007	0.00014
2.05396					
R24	2.59313	0.00008	0.00023	0.00003	0.00026
2.59339					
R25	2.05432	0.00002	0.00009	-0.00001	0.00007
2.05440					
R26	2.04771	0.00004	-0.00001	0.00013	0.00012
2.04783					
R27	2.07428	-0.00002	0.00048	-0.00016	0.00032
2.07460					
R28	2.05844	0.00011	0.00051	-0.00016	0.00035
2.05879					
R29	2.07441	-0.00013	-0.00092	-0.00016	-0.00109
2.07332					
A1	2.09068	-0.00001	-0.00010	0.00004	-0.00007
2.09061					
A2	2.10134	0.00005	0.00039	-0.00005	0.00034
2.10168					
A3	2.09117	-0.00005	-0.00029	0.00002	-0.00028
2.09089					
A4	2.11524	0.00000	0.00007	-0.00006	0.00001
2.11525					
A5	2.10374	0.00006	0.00031	0.00011	0.00042
2.10416					
A6	2.06420	-0.00006	-0.00038	-0.00005	-0.00043
2.06377					
A7	2.08411	0.00001	0.00004	0.00001	0.00005
2.08417					

A8	2.11684	-0.00007	-0.00036	-0.00002	-0.00039
2.11645					
A9	2.08223	0.00006	0.00032	0.00001	0.00033
2.08257					
A10	2.04791	-0.00002	-0.00029	0.00011	-0.00018
2.04773					
A11	2.09900	-0.00007	-0.00034	0.00000	-0.00034
2.09867					
A12	2.13627	0.00009	0.00063	-0.00011	0.00051
2.13678					
A13	2.12232	0.00000	0.00016	-0.00013	0.00004
2.12235					
A14	2.08504	0.00004	0.00020	0.00005	0.00025
2.08529					
A15	2.07583	-0.00004	-0.00036	0.00007	-0.00029
2.07554					
A16	2.10611	0.00002	0.00011	0.00003	0.00014
2.10624					
A17	2.08635	-0.00004	-0.00023	0.00007	-0.00016
2.08619					
A18	2.09072	0.00001	0.00012	-0.00009	0.00002
2.09075					
A19	2.11916	0.00000	0.00001	-0.00001	0.00001
2.11917					
A20	2.08272	-0.00001	-0.00008	-0.00002	-0.00010
2.08262					
A21	2.08130	0.00001	0.00006	0.00003	0.00010
2.08140					
A22	2.08838	-0.00001	-0.00013	0.00003	-0.00009
2.08829					
A23	2.06604	0.00034	0.00218	-0.00002	0.00216
2.06820					
A24	2.12877	-0.00032	-0.00206	-0.00001	-0.00207
2.12669					
A25	2.08710	0.00007	0.00038	-0.00003	0.00035
2.08745					
A26	2.15757	-0.00014	-0.00066	-0.00003	-0.00070
2.15687					
A27	2.03852	0.00007	0.00028	0.00007	0.00034
2.03886					
A28	2.09049	-0.00005	-0.00029	0.00000	-0.00029
2.09021					
A29	2.10631	0.00006	0.00035	-0.00004	0.00031
2.10662					
A30	2.08638	-0.00002	-0.00006	0.00004	-0.00002
2.08636					
A31	2.06140	-0.00005	-0.00019	-0.00005	-0.00024
2.06116					
A32	2.11779	-0.00001	-0.00010	-0.00005	-0.00015
2.11764					
A33	2.10399	0.00006	0.00029	0.00010	0.00039
2.10438					

A34	2.08768	0.00002	0.00012	0.00003	0.00015
2.08783					
A35	2.10307	0.00004	0.00028	-0.00005	0.00023
2.10331					
A36	2.09244	-0.00006	-0.00040	0.00001	-0.00038
2.09205					
A37	2.10857	-0.00001	-0.00006	0.00003	-0.00002
2.10855					
A38	2.08638	-0.00003	-0.00024	0.00006	-0.00018
2.08620					
A39	2.08824	0.00004	0.00030	-0.00010	0.00021
2.08844					
A40	2.12744	-0.00005	-0.00020	-0.00011	-0.00031
2.12714					
A41	2.09103	-0.00003	-0.00021	0.00005	-0.00016
2.09087					
A42	2.06471	0.00008	0.00040	0.00007	0.00047
2.06518					
A43	1.93979	0.00012	0.00149	0.00049	0.00198
1.94177					
A44	1.97491	-0.00012	-0.00160	-0.00016	-0.00176
1.97315					
A45	1.93953	0.00008	0.00071	-0.00002	0.00069
1.94022					
A46	1.86848	-0.00005	0.00062	-0.00049	0.00013
1.86862					
A47	1.86846	-0.00002	0.00039	0.00003	0.00043
1.86889					
A48	1.86733	-0.00001	-0.00163	0.00012	-0.00150
1.86584					
D1	0.00001	0.00000	-0.00003	-0.00021	-0.00024	-
0.00022					
D2	3.14156	0.00000	-0.00074	-0.00012	-0.00085
3.14071					
D3	3.14153	0.00000	0.00055	-0.00016	0.00039	-
3.14127					
D4	-0.00011	0.00000	-0.00016	-0.00007	-0.00023	-
0.00034					
D5	0.00011	0.00000	0.00113	0.00014	0.00126
0.00138					
D6	-3.14133	0.00000	0.00117	0.00023	0.00139	-
3.13993					
D7	-3.14140	0.00000	0.00055	0.00009	0.00064	-
3.14076					
D8	0.00034	0.00000	0.00059	0.00018	0.00077
0.00111					
D9	-0.00022	0.00000	-0.00160	0.00010	-0.00150	-
0.00172					
D10	3.14133	0.00000	-0.00184	0.00005	-0.00178
3.13955					
D11	3.14142	0.00000	-0.00091	0.00001	-0.00089
3.14052					

This journal is © The Royal Society of Chemistry 2014

D12	-0.00022	0.00000	-0.00114	-0.00004	-0.00117	-0.00139
D13	0.00030	0.00000	0.00209	0.00008	0.00217	0.00247
D14	-3.14101	-0.00001	0.00116	-0.00044	0.00072	-3.14029
D15	-3.14126	0.00000	0.00232	0.00012	0.00244	-3.13881
D16	0.00062	-0.00001	0.00139	-0.00039	0.00100	0.00162
D17	-3.14122	0.00000	0.00195	0.00054	0.00249	-3.13873
D18	0.00026	0.00000	0.00073	0.00047	0.00120	0.00146
D19	0.00033	0.00001	0.00172	0.00049	0.00221	0.00254
D20	-3.14138	0.00000	0.00049	0.00042	0.00092	-3.14046
D21	-0.00018	0.00000	-0.00105	-0.00015	-0.00120	-0.00138
D22	3.14104	0.00000	-0.00291	0.00003	-0.00288	3.13815
D23	3.14112	0.00001	-0.00009	0.00037	0.00028	3.14140
D24	-0.00085	0.00001	-0.00195	0.00055	-0.00140	-0.00225
D25	-0.00176	0.00001	-0.00436	0.00005	-0.00431	-0.00607
D26	3.14040	0.00000	-0.00287	-0.00034	-0.00323	3.13717
D27	3.14014	0.00000	-0.00535	-0.00049	-0.00584	3.13430
D28	-0.00090	-0.00001	-0.00386	-0.00088	-0.00475	-0.00564
D29	-0.00003	0.00000	-0.00056	0.00005	-0.00051	-0.00054
D30	3.14141	0.00000	-0.00060	-0.00004	-0.00064	3.14077
D31	-3.14124	0.00000	0.00129	-0.00013	0.00116	-3.14008
D32	0.00020	0.00000	0.00125	-0.00022	0.00103	0.00123
D33	-0.00014	-0.00001	-0.00179	-0.00025	-0.00204	-0.00218
D34	3.14097	0.00000	-0.00195	-0.00023	-0.00218	3.13879
D35	3.14157	0.00000	-0.00057	-0.00019	-0.00075	3.14081
D36	-0.00051	0.00001	-0.00073	-0.00016	-0.00089	-0.00140
D37	0.00194	-0.00001	0.00428	0.00018	0.00446	0.00640

D38	-3.13877	-0.00002	0.00524	-0.00026	0.00498	-3.13378
D39	-3.14024	0.00000	0.00275	0.00060	0.00334	-3.13690
D40	0.00225	-0.00002	0.00371	0.00015	0.00386	0.00610
D41	1.04739	0.00006	0.04120	-0.00079	0.04040	1.08779
D42	-3.13283	-0.00001	0.04195	-0.00118	0.04077	-3.09206
D43	-1.03154	-0.00005	0.03924	-0.00114	0.03810	-0.99344
D44	-2.09363	0.00006	0.04271	-0.00120	0.04151	-2.05211
D45	0.00934	-0.00001	0.04346	-0.00159	0.04188	0.05122
D46	2.11063	-0.00005	0.04076	-0.00155	0.03921	2.14984
D47	-0.00101	0.00001	-0.00124	-0.00009	-0.00133	-0.00234
D48	3.14107	0.00000	-0.00108	-0.00012	-0.00120	3.13987
D49	3.13976	0.00002	-0.00214	0.00032	-0.00182	3.13794
D50	-0.00135	0.00001	-0.00198	0.00029	-0.00169	-0.00304
D51	-3.14143	0.00000	0.00005	0.00028	0.00033	-3.14110
D52	0.00105	0.00000	0.00205	-0.00010	0.00194	0.00299
D53	0.00103	-0.00001	0.00099	-0.00015	0.00084	0.00187
D54	-3.13968	-0.00002	0.00298	-0.00053	0.00245	-3.13723
D55	0.00105	-0.00001	0.00090	-0.00010	0.00081	0.00186
D56	-3.14028	-0.00001	0.00168	-0.00035	0.00134	-3.13895
D57	-3.14102	0.00000	0.00074	-0.00007	0.00067	-3.14035
D58	0.00083	-0.00001	0.00152	-0.00032	0.00120	0.00203
D59	0.00010	0.00000	0.00003	0.00018	0.00021	0.00032
D60	3.14137	0.00000	-0.00052	0.00033	-0.00019	3.14118
D61	-3.14123	0.00000	0.00083	-0.00007	0.00075	-3.14047
D62	0.00004	0.00000	0.00028	0.00007	0.00035	0.00039
D63	-0.00046	0.00000	-0.00107	-0.00003	-0.00110	-0.00157

```
   D64        3.14078   0.00000  -0.00119  -0.00003  -0.00122
3.13955
   D65        3.14146   0.00000  -0.00052  -0.00018  -0.00070
3.14075
   D66       -0.00049   0.00000  -0.00064  -0.00018  -0.00082  -
0.00131
   D67       -0.00014   0.00001   0.00053   0.00002   0.00055
0.00041
   D68        3.14059   0.00001  -0.00144   0.00040  -0.00104
3.13955
   D69       -3.14137   0.00000   0.00065   0.00002   0.00067  -
3.14071
   D70       -0.00065   0.00001  -0.00132   0.00040  -0.00092  -
0.00157
         Item               Value     Threshold  Converged?
 Maximum Force            0.000338     0.000450     YES
 RMS     Force            0.000057     0.000300     YES
 Maximum Displacement     0.090406     0.001800     NO
 RMS     Displacement     0.011807     0.001200     NO
 Predicted change in Energy=-5.345672D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793456   -5.418529    0.015952
      2          6           0       -3.422757   -5.391895    0.008142
      3          6           0       -2.705580   -4.153729   -0.003832
      4          6           0       -3.439046   -2.908861   -0.009928
      5          6           0       -4.871113   -2.988350   -0.000355
      6          6           0       -5.524882   -4.196311    0.012429
      7          6           0       -1.307248   -4.124867   -0.009372
      8          6           0       -2.746089   -1.671490   -0.023397
      9          6           0       -1.328791   -1.661549   -0.023383
     10          6           0       -0.603529   -2.917522   -0.017656
     11          6           0        0.828490   -2.905921   -0.019797
     12          1           0        1.348622   -3.861475   -0.016582
     13          6           0        1.531141   -1.730367   -0.024792
     14          6           0        0.829345   -0.490398   -0.027553
     15          6           0       -0.542665   -0.459215   -0.027115
     16          1           0       -0.754625   -5.062700   -0.005858
     17          1           0       -5.325415   -6.366365    0.025330
     18          1           0       -2.851473   -6.317802    0.011545
     19          1           0       -5.456339   -2.075236   -0.001286
     20          1           0       -6.611708   -4.222226    0.020221
     21          1           0        2.618027   -1.737139   -0.025973
     22          1           0        1.388628    0.441842   -0.029591
     23          1           0       -1.035043    0.506134   -0.027337
```

24	6	0	-3.554265	-0.390778	-0.035277
25	1	0	-4.167301	-0.298598	0.870768
26	1	0	-2.935246	0.503765	-0.094812
27	1	0	-4.239111	-0.362429	-0.891974

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370980	0.000000			
3	C	2.441176	1.430923	0.000000		
4	C	2.851934	2.483153	1.444890	0.000000	
5	C	2.431474	2.806214	2.459198	1.434303	0.000000
6	C	1.424364	2.418341	2.819671	2.451272	1.373589
7	C	3.718582	2.465978	1.398641	2.454228	3.740707
8	C	4.270078	3.781572	2.482647	1.418259	2.500075
9	C	5.110807	4.277986	2.847260	2.451356	3.782720
10	C	4.879719	3.751164	2.438650	2.835541	4.268206
11	C	6.157983	4.924830	3.747923	4.267549	5.700232
12	H	6.336450	5.010874	4.064742	4.881525	6.280742
13	C	7.321525	6.160274	4.880873	5.108016	6.524720
14	C	7.476915	6.488938	5.090801	4.905960	6.223803
15	C	6.531913	5.712050	4.281143	3.793427	5.013253
16	H	4.054535	2.688400	2.152314	3.441679	4.609602
17	H	1.086950	2.137755	3.429307	3.938777	3.408524
18	H	2.140095	1.087970	2.169039	3.459274	3.894141
19	H	3.408419	3.890472	3.447726	2.182768	1.084558
20	H	2.176511	3.396716	3.906803	3.433893	2.133670
21	H	8.275534	7.060416	5.846467	6.169386	7.592983
22	H	8.518462	7.561966	6.154874	5.876567	7.138026
23	H	7.016351	6.363111	4.950310	4.176329	5.189179
24	C	5.178465	5.003035	3.857598	2.520845	2.912505
25	H	5.228430	5.219209	4.214688	2.849465	2.913584
26	H	6.207961	5.916678	4.664041	3.450658	3.993916
27	H	5.166796	5.174184	4.185030	2.811126	2.844271

		6	7	8	9	10
6	C	0.000000				
7	C	4.218296	0.000000			
8	C	3.754689	2.844209	0.000000		
9	C	4.902395	2.463452	1.417333	0.000000	
10	C	5.084872	1.397487	2.478547	1.450347	0.000000
11	C	6.483169	2.459129	3.781726	2.490449	1.432068
12	H	6.881716	2.668909	4.643571	3.465294	2.168397
13	C	7.474605	3.713532	4.277636	2.860760	2.442581
14	C	7.356058	4.216008	3.765465	2.455436	2.818538
15	C	6.228157	3.744584	2.514897	1.436530	2.459079
16	H	4.848332	1.088547	3.932753	3.449318	2.150524
17	H	2.179240	4.601216	5.356972	6.173384	5.847441
18	H	3.412893	2.682169	4.647638	4.899027	4.076273
19	H	2.122226	4.627744	2.740247	4.148286	4.925391
20	H	1.087163	5.305436	4.631540	5.870961	6.148325
21	H	8.506231	4.594486	5.364518	3.947542	3.431005
22	H	8.325313	5.303111	4.643500	3.436373	3.905657

This journal is © The Royal Society of Chemistry 2014

23	H	6.501786	4.639029	2.769430	2.187499	3.450756
24	C	4.285754	4.358117	1.514435	2.562759	3.884790
25	H	4.215677	4.857457	2.168918	3.273267	4.510935
26	H	5.367348	4.907333	2.184631	2.697107	4.141022
27	H	4.143647	4.850851	2.167298	3.303351	4.528840

		11	12	13	14	15
11	C	0.000000				
12	H	1.087949	0.000000			
13	C	1.369551	2.138926	0.000000		
14	C	2.415535	3.410855	1.424798	0.000000	
15	C	2.804726	3.892616	2.432387	1.372364	0.000000
16	H	2.675470	2.422128	4.040980	4.838943	4.608411
17	H	7.060259	7.128745	8.276917	8.509457	7.600781
18	H	5.018370	4.865710	6.344539	6.892647	6.297232
19	H	6.339515	7.035509	6.996025	6.482455	5.172658
20	H	7.555846	7.968586	8.515714	8.324548	7.141133
21	H	2.137412	2.474728	1.086907	2.180309	3.409261
22	H	3.394314	4.303523	2.176885	1.087140	2.131150
23	H	3.887792	4.975739	3.404004	2.114005	1.083667
24	C	5.053190	6.007029	5.258894	4.384749	3.012389
25	H	5.705187	6.626228	5.943419	5.080378	3.737644
26	H	5.079104	6.116615	4.994483	3.894231	2.579992
27	H	5.736778	6.650744	5.993252	5.143233	3.797507

		16	17	18	19	20
16	H	0.000000				
17	H	4.753172	0.000000			
18	H	2.443841	2.474457	0.000000		
19	H	5.570554	4.293208	4.978438	0.000000	
20	H	5.917136	2.500381	4.304751	2.438218	0.000000
21	H	4.736510	9.194054	7.134375	8.081479	9.558546
22	H	5.907120	9.562064	7.979532	7.293151	9.260744
23	H	5.575930	8.101932	7.061659	5.119767	7.311556
24	C	5.446623	6.232839	5.968728	2.540953	4.902146
25	H	5.925495	6.234885	6.220971	2.361893	4.700363
26	H	5.979009	7.275027	6.822910	3.607756	5.988706
27	H	5.917719	6.169988	6.181290	2.282254	4.621619

		21	22	23	24	25
21	H	0.000000				
22	H	2.501878	0.000000			
23	H	4.286863	2.424524	0.000000		
24	C	6.317433	5.012532	2.674134	0.000000	
25	H	6.993870	5.676904	3.356371	1.097829	0.000000
26	H	5.988759	4.324809	1.901403	1.089466	1.759002
27	H	7.046994	5.749956	3.430459	1.097154	1.765359

		26	27
26	H	0.000000	
27	H	1.756651	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1

This journal is © The Royal Society of Chemistry 2014

```
 Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.652294   -1.004899    0.003343
      2          6           0       -2.452754   -1.668728   -0.001323
      3          6           0       -1.211603   -0.956629   -0.002834
      4          6           0       -1.222459    0.488220   -0.001542
      5          6           0       -2.501599    1.137055    0.004375
      6          6           0       -3.672747    0.419313    0.007050
      7          6           0        0.012953   -1.632389   -0.005155
      8          6           0       -0.002657    1.211776   -0.004605
      9          6           0        1.228799    0.510109   -0.001468
     10          6           0        1.226992   -0.940236   -0.003227
     11          6           0        2.472032   -1.647832   -0.002201
     12          1           0        2.443271   -2.735397   -0.004750
     13          6           0        3.669197   -0.982671    0.002785
     14          6           0        3.683276    0.442050    0.007445
     15          6           0        2.511615    1.156606    0.005153
     16          1           0        0.021188   -2.720903   -0.007207
     17          1           0       -4.587660   -1.558569    0.004748
     18          1           0       -2.422394   -2.756273   -0.003360
     19          1           0       -2.550449    2.220504    0.008762
     20          1           0       -4.626274    0.941503    0.012315
     21          1           0        4.606359   -1.533210    0.003895
     22          1           0        4.634431    0.968493    0.013326
     23          1           0        2.569285    2.238722    0.010825
     24          6           0       -0.060169    2.725112   -0.009000
     25          1           0       -0.549433    3.107429    0.896364
     26          1           0        0.924104    3.189294   -0.060756
     27          1           0       -0.633913    3.097266   -0.866943
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3942556      0.4478372
0.3396799
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9238090314 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
```

```
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860688757     A.U. after   10 cycles
             Convg  =    0.9299D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
```

```
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000017910   -0.000011267    0.000003610
      2        6           0.000012965   -0.000016698   -0.000004641
      3        6           0.000012833    0.000002094    0.000004030
      4        6           0.000001772    0.000022049    0.000019337
      5        6           0.000036244    0.000052353    0.000004097
      6        6          -0.000011437   -0.000005709   -0.000000783
      7        6           0.000005333   -0.000002394   -0.000003806
      8        6          -0.000043163   -0.000003638   -0.000046225
      9        6           0.000006285    0.000034563   -0.000010715
     10        6           0.000005531   -0.000023642    0.000009002
     11        6           0.000018445   -0.000008997   -0.000006912
     12        1          -0.000015165    0.000007217    0.000002079
     13        6           0.000014030   -0.000004316    0.000003062
     14        6          -0.000008019    0.000005414   -0.000001911
     15        6           0.000049690    0.000009076    0.000000818
     16        1          -0.000007359    0.000010023    0.000007372
     17        1          -0.000005345    0.000015339    0.000003675
     18        1           0.000000995    0.000016123   -0.000000134
     19        1           0.000017129    0.000038510    0.000005325
     20        1           0.000006615   -0.000008466   -0.000002428
     21        1          -0.000009952    0.000012134    0.000002647
     22        1           0.000003976   -0.000009793   -0.000004587
     23        1           0.000067037   -0.000031106    0.000004749
     24        6           0.000029152   -0.000018661    0.000012490
     25        1          -0.000065442   -0.000046769    0.000053558
     26        1          -0.000081509   -0.000010112   -0.000013330
     27        1          -0.000022729   -0.000023328   -0.000040379
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000081509 RMS     0.000023511


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000358100 RMS     0.000055913
 Search for a local minimum.
 Step number  47 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   35   34   36   37
38
                                                     39   40   41   42
43
                                                     44   45   46   47
 DE=  7.77D-07 DEPred=-5.35D-07 R=-1.45D+00
```

This journal is © The Royal Society of Chemistry 2014

```
 Trust test=-1.45D+00 RLast= 1.00D-01 DXMaxT set to 8.41D-02
     Eigenvalues ---    0.00027   0.00823   0.01294   0.01586
0.01726
     Eigenvalues ---    0.01770   0.01807   0.01821   0.01917
0.01934
     Eigenvalues ---    0.01972   0.01981   0.02016   0.02061
0.02102
     Eigenvalues ---    0.02109   0.02146   0.02191   0.02210
0.02226
     Eigenvalues ---    0.02338   0.02351   0.05311   0.06623
0.10512
     Eigenvalues ---    0.11537   0.15297   0.15532   0.15725
0.15942
     Eigenvalues ---    0.15999   0.16002   0.16004   0.16006
0.16078
     Eigenvalues ---    0.16311   0.19462   0.21987   0.22044
0.22461
     Eigenvalues ---    0.22678   0.23083   0.24209   0.24435
0.24870
     Eigenvalues ---    0.26434   0.28616   0.29900   0.31669
0.32910
     Eigenvalues ---    0.33576   0.33601   0.33631   0.33682
0.33684
     Eigenvalues ---    0.33746   0.34188   0.34295   0.35576
0.36816
     Eigenvalues ---    0.37413   0.37859   0.38161   0.39565
0.40320
     Eigenvalues ---    0.40710   0.40928   0.41995   0.44558
0.45831
     Eigenvalues ---    0.49079   0.49840   0.51121   0.51250
0.57557
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    47   46   45   44
43
 RFO step:  Lambda=-6.98080731D-07.
 DIIS coeffs:      0.47223      0.64737      0.12239     -0.36774
0.12574
 Iteration  1 RMS(Cart)=  0.00792464 RMS(Int)=  0.00008963
 Iteration  2 RMS(Cart)=  0.00009296 RMS(Int)=  0.00000063
 Iteration  3 RMS(Cart)=  0.00000001 RMS(Int)=  0.00000063
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59078   0.00004   0.00005   0.00004   0.00009
2.59087
    R2        2.69166   0.00001   0.00001  -0.00005  -0.00004
2.69162
    R3        2.05404  -0.00001  -0.00005   0.00001  -0.00004
2.05400
    R4        2.70405   0.00001  -0.00004  -0.00001  -0.00005
2.70401
    R5        2.05597  -0.00001  -0.00001  -0.00002  -0.00003
2.05593
    R6        2.73045  -0.00005  -0.00013   0.00005  -0.00009
2.73036
    R7        2.64305  -0.00003   0.00005  -0.00006   0.00000
2.64305
    R8        2.71044  -0.00006   0.00005  -0.00014  -0.00009
2.71035
    R9        2.68012  -0.00013   0.00014  -0.00015  -0.00001
2.68011
   R10        2.59571   0.00001  -0.00004   0.00010   0.00005
2.59576
   R11        2.04952   0.00002  -0.00008   0.00006  -0.00002
2.04949
   R12        2.05444  -0.00001  -0.00001  -0.00001  -0.00002
2.05442
   R13        2.64087   0.00001  -0.00014   0.00008  -0.00006
2.64081
   R14        2.05706  -0.00001  -0.00001  -0.00002  -0.00003
2.05702
   R15        2.67837   0.00016  -0.00031   0.00036   0.00005
2.67842
   R16        2.86187  -0.00001   0.00023  -0.00032  -0.00009
2.86178
```

This journal is © The Royal Society of Chemistry 2014

R17	2.74076	0.00008	0.00021	0.00002	0.00023
2.74099					
R18	2.71465	0.00007	0.00012	-0.00004	0.00008
2.71473					
R19	2.70622	0.00001	0.00008	-0.00006	0.00002
2.70623					
R20	2.05593	-0.00001	-0.00001	-0.00002	-0.00003
2.05589					
R21	2.58808	-0.00002	-0.00003	0.00002	-0.00001
2.58807					
R22	2.69248	-0.00003	0.00010	-0.00012	-0.00002
2.69245					
R23	2.05396	-0.00001	-0.00007	0.00002	-0.00004
2.05391					
R24	2.59339	0.00000	-0.00012	0.00010	-0.00002
2.59337					
R25	2.05440	-0.00001	-0.00001	-0.00001	-0.00002
2.05438					
R26	2.04783	-0.00006	-0.00009	-0.00002	-0.00011
2.04772					
R27	2.07460	0.00008	-0.00019	0.00003	-0.00016
2.07444					
R28	2.05879	-0.00005	-0.00011	0.00006	-0.00005
2.05874					
R29	2.07332	0.00004	0.00050	-0.00002	0.00049
2.07381					
A1	2.09061	0.00000	0.00001	-0.00002	-0.00001
2.09060					
A2	2.10168	0.00001	-0.00009	0.00015	0.00005
2.10173					
A3	2.09089	-0.00001	0.00009	-0.00013	-0.00004
2.09085					
A4	2.11525	-0.00001	0.00003	-0.00004	-0.00001
2.11524					
A5	2.10416	0.00002	-0.00020	0.00023	0.00003
2.10419					
A6	2.06377	0.00000	0.00017	-0.00019	-0.00002
2.06375					
A7	2.08417	-0.00002	-0.00003	0.00002	-0.00001
2.08416					
A8	2.11645	0.00005	0.00015	-0.00003	0.00012
2.11657					
A9	2.08257	-0.00003	-0.00012	0.00001	-0.00011
2.08246					
A10	2.04773	0.00006	0.00003	0.00004	0.00007
2.04780					
A11	2.09867	0.00009	0.00012	0.00005	0.00017
2.09884					
A12	2.13678	-0.00015	-0.00015	-0.00009	-0.00024
2.13654					
A13	2.12235	-0.00002	0.00004	-0.00006	-0.00002
2.12233					

This journal is © The Royal Society of Chemistry 2014

A14	2.08529	-0.00003	-0.00014	0.00012	-0.00002
2.08527					
A15	2.07554	0.00004	0.00011	-0.00006	0.00004
2.07558					
A16	2.10624	-0.00001	-0.00007	0.00006	-0.00001
2.10623					
A17	2.08619	0.00000	0.00002	-0.00005	-0.00003
2.08616					
A18	2.09075	0.00001	0.00005	-0.00001	0.00004
2.09079					
A19	2.11917	0.00000	0.00000	0.00003	0.00002
2.11920					
A20	2.08262	0.00000	0.00004	-0.00005	-0.00001
2.08261					
A21	2.08140	0.00000	-0.00004	0.00002	-0.00001
2.08138					
A22	2.08829	0.00000	0.00002	-0.00002	-0.00001
2.08829					
A23	2.06820	-0.00035	-0.00085	-0.00006	-0.00091
2.06729					
A24	2.12669	0.00036	0.00084	0.00009	0.00092
2.12761					
A25	2.08745	-0.00009	-0.00012	-0.00005	-0.00017
2.08728					
A26	2.15687	0.00018	0.00030	0.00009	0.00039
2.15726					
A27	2.03886	-0.00008	-0.00018	-0.00004	-0.00022
2.03864					
A28	2.09021	0.00003	0.00011	-0.00001	0.00010
2.09031					
A29	2.10662	-0.00006	-0.00009	-0.00007	-0.00016
2.10646					
A30	2.08636	0.00003	-0.00001	0.00008	0.00006
2.08642					
A31	2.06116	-0.00002	0.00009	-0.00019	-0.00010
2.06106					
A32	2.11764	0.00001	0.00010	-0.00004	0.00006
2.11770					
A33	2.10438	0.00000	-0.00019	0.00023	0.00004
2.10442					
A34	2.08783	-0.00001	-0.00007	-0.00001	-0.00008
2.08775					
A35	2.10331	0.00002	-0.00006	0.00015	0.00010
2.10340					
A36	2.09205	-0.00001	0.00012	-0.00014	-0.00002
2.09203					
A37	2.10855	0.00002	-0.00002	0.00007	0.00005
2.10860					
A38	2.08620	-0.00002	0.00001	-0.00006	-0.00005
2.08615					
A39	2.08844	0.00000	0.00000	-0.00001	-0.00001
2.08844					

This journal is © The Royal Society of Chemistry 2014

A40	2.12714	0.00003	0.00018	-0.00005	0.00012	2.12726
A41	2.09087	0.00003	0.00000	0.00011	0.00011	2.09098
A42	2.06518	-0.00006	-0.00018	-0.00005	-0.00023	2.06495
A43	1.94177	-0.00006	-0.00109	0.00018	-0.00090	1.94087
A44	1.97315	0.00012	0.00073	0.00017	0.00090	1.97405
A45	1.94022	-0.00006	-0.00014	0.00030	0.00015	1.94038
A46	1.86862	0.00001	-0.00015	-0.00052	-0.00067	1.86794
A47	1.86889	0.00001	-0.00016	-0.00006	-0.00021	1.86868
A48	1.86584	-0.00002	0.00083	-0.00012	0.00071	1.86655
D1	-0.00022	0.00000	0.00024	-0.00007	0.00017	-0.00006
D2	3.14071	0.00000	0.00045	0.00013	0.00058	3.14129
D3	-3.14127	0.00000	-0.00006	-0.00012	-0.00018	-3.14144
D4	-0.00034	0.00000	0.00015	0.00008	0.00023	-0.00010
D5	0.00138	0.00000	-0.00053	-0.00027	-0.00080	0.00058
D6	-3.13993	0.00000	-0.00064	-0.00035	-0.00098	-3.14092
D7	-3.14076	0.00000	-0.00024	-0.00021	-0.00046	-3.14122
D8	0.00111	0.00000	-0.00034	-0.00030	-0.00064	0.00047
D9	-0.00172	0.00000	0.00055	0.00041	0.00096	-0.00076
D10	3.13955	0.00000	0.00076	0.00041	0.00117	3.14072
D11	3.14052	0.00000	0.00034	0.00021	0.00056	3.14108
D12	-0.00139	0.00000	0.00055	0.00021	0.00076	-0.00063
D13	0.00247	0.00000	-0.00101	-0.00042	-0.00143	0.00103
D14	-3.14029	0.00000	-0.00019	-0.00042	-0.00061	-3.14090
D15	-3.13881	0.00001	-0.00122	-0.00042	-0.00163	-3.14045
D16	0.00162	0.00000	-0.00039	-0.00042	-0.00081	0.00081
D17	-3.13873	0.00000	-0.00145	-0.00036	-0.00181	-3.14055

This journal is © The Royal Society of Chemistry 2014

D18	0.00146	0.00000	-0.00053	-0.00041	-0.00094	0.00052
D19	0.00254	0.00000	-0.00124	-0.00037	-0.00160	0.00093
D20	-3.14046	0.00000	-0.00033	-0.00041	-0.00073	-3.14119
D21	-0.00138	0.00000	0.00074	0.00010	0.00083	-0.00054
D22	3.13815	0.00000	0.00137	0.00062	0.00198	3.14014
D23	3.14140	0.00000	-0.00010	0.00010	-0.00001	3.14140
D24	-0.00225	0.00000	0.00053	0.00062	0.00114	-0.00111
D25	-0.00607	0.00000	0.00223	0.00121	0.00345	-0.00262
D26	3.13717	0.00001	0.00133	0.00131	0.00264	3.13981
D27	3.13430	-0.00001	0.00310	0.00121	0.00431	3.13861
D28	-0.00564	0.00000	0.00220	0.00131	0.00350	-0.00214
D29	-0.00054	0.00000	0.00003	0.00025	0.00028	-0.00026
D30	3.14077	0.00000	0.00013	0.00033	0.00046	3.14123
D31	-3.14008	0.00000	-0.00060	-0.00027	-0.00087	-3.14095
D32	0.00123	0.00000	-0.00050	-0.00019	-0.00069	0.00054
D33	-0.00218	0.00000	0.00101	0.00034	0.00135	-0.00083
D34	3.13879	0.00000	0.00124	0.00044	0.00167	3.14047
D35	3.14081	0.00000	0.00010	0.00038	0.00048	3.14129
D36	-0.00140	0.00000	0.00033	0.00048	0.00080	-0.00060
D37	0.00640	0.00000	-0.00245	-0.00123	-0.00368	0.00271
D38	-3.13378	0.00001	-0.00286	-0.00158	-0.00444	-3.13823
D39	-3.13690	-0.00001	-0.00152	-0.00133	-0.00285	-3.13975
D40	0.00610	0.00000	-0.00192	-0.00168	-0.00361	0.00250
D41	1.08779	-0.00005	-0.02246	-0.00335	-0.02582	1.06197
D42	-3.09206	0.00000	-0.02293	-0.00378	-0.02671	-3.11877
D43	-0.99344	0.00001	-0.02145	-0.00360	-0.02505	-1.01849

This journal is © The Royal Society of Chemistry 2014

D44	-2.05211	-0.00004	-0.02339	-0.00326	-0.02665	-2.07876
D45	0.05122	0.00001	-0.02386	-0.00368	-0.02754	0.02368
D46	2.14984	0.00002	-0.02238	-0.00351	-0.02588	2.12396
D47	-0.00234	0.00000	0.00086	0.00046	0.00133	-0.00101
D48	3.13987	0.00000	0.00063	0.00037	0.00100	3.14087
D49	3.13794	0.00000	0.00124	0.00079	0.00203	3.13997
D50	-0.00304	0.00000	0.00101	0.00070	0.00171	-0.00133
D51	-3.14110	0.00000	-0.00037	0.00003	-0.00035	-3.14144
D52	0.00299	0.00000	-0.00109	-0.00059	-0.00167	0.00132
D53	0.00187	0.00000	-0.00077	-0.00031	-0.00108	0.00079
D54	-3.13723	0.00000	-0.00149	-0.00093	-0.00241	-3.13964
D55	0.00186	0.00000	-0.00055	-0.00044	-0.00099	0.00087
D56	-3.13895	0.00000	-0.00074	-0.00068	-0.00142	-3.14037
D57	-3.14035	0.00000	-0.00032	-0.00034	-0.00066	-3.14102
D58	0.00203	0.00000	-0.00051	-0.00059	-0.00109	0.00093
D59	0.00032	0.00000	-0.00029	0.00005	-0.00024	0.00008
D60	3.14118	0.00000	-0.00004	0.00021	0.00016	3.14134
D61	-3.14047	0.00000	-0.00048	-0.00020	-0.00068	-3.14115
D62	0.00039	0.00000	-0.00024	-0.00004	-0.00028	0.00011
D63	-0.00157	0.00000	0.00056	0.00035	0.00091	-0.00066
D64	3.13955	0.00000	0.00070	0.00049	0.00119	3.14074
D65	3.14075	0.00000	0.00031	0.00020	0.00051	3.14127
D66	-0.00131	0.00000	0.00045	0.00034	0.00079	-0.00052
D67	0.00041	0.00000	0.00000	-0.00021	-0.00022	0.00020
D68	3.13955	0.00000	0.00070	0.00039	0.00109	3.14064
D69	-3.14071	0.00000	-0.00014	-0.00035	-0.00049	-3.14120

```
   D70       -0.00157   0.00000   0.00056   0.00025   0.00081  -
0.00076
         Item               Value     Threshold  Converged?
 Maximum Force            0.000358     0.000450     YES
 RMS     Force            0.000056     0.000300     YES
 Maximum Displacement     0.061576     0.001800     NO
 RMS     Displacement     0.007925     0.001200     NO
 Predicted change in Energy=-1.454052D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793477   -5.418127    0.015675
      2          6           0       -3.422717   -5.391636    0.010191
      3          6           0       -2.705420   -4.153564   -0.001408
      4          6           0       -3.438748   -2.908671   -0.008405
      5          6           0       -4.870794   -2.987949   -0.001898
      6          6           0       -5.524750   -4.195851    0.009854
      7          6           0       -1.307086   -4.124678   -0.005975
      8          6           0       -2.745884   -1.671241   -0.020773
      9          6           0       -1.328561   -1.661225   -0.023015
     10          6           0       -0.603375   -2.917377   -0.016051
     11          6           0        0.828653   -2.906031   -0.019220
     12          1           0        1.348516   -3.861706   -0.014403
     13          6           0        1.531573   -1.730665   -0.027632
     14          6           0        0.829973   -0.490609   -0.033283
     15          6           0       -0.542017   -0.459134   -0.031174
     16          1           0       -0.754463   -5.062486   -0.001087
     17          1           0       -5.325589   -6.365856    0.024627
     18          1           0       -2.851517   -6.317568    0.014821
     19          1           0       -5.455867   -2.074759   -0.005464
     20          1           0       -6.611584   -4.221683    0.014878
     21          1           0        2.618434   -1.737592   -0.029706
     22          1           0        1.389434    0.441495   -0.039154
     23          1           0       -1.033946    0.506371   -0.034758
     24          6           0       -3.555298   -0.391345   -0.030135
     25          1           0       -4.186872   -0.314435    0.864429
     26          1           0       -2.937154    0.505171   -0.062227
     27          1           0       -4.222894   -0.350863   -0.900188
 ---------------------------------------------------------------------
                   Distance matrix (angstroms):
                    1          2          3          4          5
    1  C    0.000000
    2  C    1.371027   0.000000
    3  C    2.441187   1.430899   0.000000
    4  C    2.851884   2.483086   1.444845   0.000000
    5  C    2.431471   2.806205   2.459168   1.434254   0.000000
```

This journal is © The Royal Society of Chemistry 2014

6	C	1.424343	2.418356	2.819670	2.451238	1.373616
7	C	3.718656	2.466038	1.398640	2.454111	3.740613
8	C	4.270026	3.781587	2.482729	1.418255	2.499864
9	C	5.110916	4.278150	2.847449	2.451372	3.782600
10	C	4.879725	3.751178	2.438640	2.835397	4.268027
11	C	6.157937	4.924758	3.747843	4.267415	5.700062
12	H	6.336200	5.010585	4.064449	4.881209	6.280400
13	C	7.321579	6.160287	4.880906	5.108049	6.524702
14	C	7.477034	6.489017	5.090900	4.906080	6.223861
15	C	6.532130	5.712244	4.281357	3.793653	5.013390
16	H	4.054676	2.688503	2.152294	3.441563	4.609543
17	H	1.086928	2.137810	3.429315	3.938703	3.408488
18	H	2.140142	1.087953	2.168991	3.459184	3.894114
19	H	3.408419	3.890452	3.447667	2.182702	1.084546
20	H	2.176463	3.396717	3.906792	3.433865	2.133712
21	H	8.275556	7.060392	5.846464	6.169387	7.592938
22	H	8.518602	7.562054	6.154984	5.876726	7.138133
23	H	7.016858	6.363547	4.950751	4.176875	5.189678
24	C	5.177231	5.002211	3.857125	2.520116	2.910959
25	H	5.209226	5.204962	4.205150	2.837533	2.892396
26	H	6.207855	5.917208	4.664892	3.450915	3.993056
27	H	5.180882	5.184445	4.191786	2.820026	2.860232

		6	7	8	9	10
6	C	0.000000				
7	C	4.218294	0.000000			
8	C	3.754556	2.844242	0.000000		
9	C	4.902389	2.463606	1.417361	0.000000	
10	C	5.084791	1.397457	2.478553	1.450470	0.000000
11	C	6.483071	2.458995	3.781801	2.490607	1.432076
12	H	6.881426	2.668604	4.643521	3.465390	2.168326
13	C	7.474640	3.713456	4.277876	2.860981	2.442627
14	C	7.356166	4.215949	3.765741	2.455548	2.818508
15	C	6.228352	3.744620	2.515222	1.436573	2.459056
16	H	4.848382	1.088530	3.932771	3.449441	2.150475
17	H	2.179175	4.601324	5.356897	6.173496	5.847475
18	H	3.412900	2.682250	4.647664	4.899220	4.076321
19	H	2.122265	4.627586	2.739903	4.148009	4.925119
20	H	1.087153	5.305426	4.631378	5.870921	6.148231
21	H	8.506235	4.594393	5.364736	3.947739	3.431054
22	H	8.325462	5.303043	4.643797	3.436450	3.905617
23	H	6.502323	4.639186	2.770004	2.187557	3.450767
24	C	4.284227	4.358075	1.514388	2.563397	3.885214
25	H	4.193520	4.854763	2.168168	3.281973	4.515751
26	H	5.366606	4.908746	2.185194	2.698589	4.142764
27	H	4.160161	4.852138	2.167563	3.296005	4.524336

		11	12	13	14	15
11	C	0.000000				
12	H	1.087932	0.000000			
13	C	1.369545	2.138930	0.000000		
14	C	2.415463	3.410798	1.424786	0.000000	
15	C	2.804672	3.892543	2.432402	1.372353	0.000000
16	H	2.675235	2.421688	4.040755	4.838753	4.608350

17	H	7.060241	7.128532	8.276981	8.509573	7.600989
18	H	5.018306	4.865428	6.344522	6.892687	6.297393
19	H	6.339273	7.035118	6.995943	6.482445	5.172700
20	H	7.555741	7.968289	8.515750	8.324662	7.141326
21	H	2.137446	2.474830	1.086884	2.180269	3.409239
22	H	3.394231	4.303467	2.176836	1.087129	2.131127
23	H	3.887672	4.975603	3.403860	2.113803	1.083607
24	C	5.053987	6.007582	5.260232	4.386395	3.014043
25	H	5.714253	6.632948	5.958364	5.099574	3.756063
26	H	5.081284	6.118731	4.996967	3.896622	2.582156
27	H	5.729146	6.644640	5.981564	5.128598	3.783618

		16	17	18	19	20
16	H	0.000000				
17	H	4.753381	0.000000			
18	H	2.443996	2.474563	0.000000		
19	H	5.570433	4.293179	4.978402	0.000000	
20	H	5.917184	2.500271	4.304747	2.438314	0.000000
21	H	4.736261	9.194089	7.134320	8.081374	9.558552
22	H	5.906907	9.562198	7.979568	7.293204	9.260909
23	H	5.575967	8.102421	7.062023	5.120203	7.312113
24	C	5.446565	6.231509	5.968035	2.539026	4.900448
25	H	5.922376	6.214631	6.208270	2.337906	4.676276
26	H	5.980525	7.274832	6.823712	3.605992	5.987531
27	H	5.919273	6.184768	6.190274	2.300559	4.639659

		21	22	23	24	25
21	H	0.000000				
22	H	2.501789	0.000000			
23	H	4.286638	2.424252	0.000000		
24	C	6.318809	5.014387	2.676403	0.000000	
25	H	7.009782	5.699393	3.379823	1.097746	0.000000
26	H	5.991294	4.327118	1.903407	1.089437	1.758477
27	H	7.034524	5.733013	3.413680	1.097413	1.765361

		26	27
26	H	0.000000	
27	H	1.757299	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.652044	-1.005326	0.001363
2	6	0	-2.452393	-1.669065	-0.000572
3	6	0	-1.211339	-0.956846	-0.001132
4	6	0	-1.222365	0.487957	-0.000585
5	6	0	-2.501505	1.136708	0.001828
6	6	0	-3.672626	0.418867	0.002922

```
      7          6           0        0.013370   -1.632330   -0.002065
      8          6           0       -0.002774    1.211866   -0.001978
      9          6           0        1.228904    0.510525   -0.000681
     10          6           0        1.227243   -0.939943   -0.001365
     11          6           0        2.472318   -1.647494   -0.000950
     12          1           0        2.443488   -2.735043   -0.002030
     13          6           0        3.669500   -0.982357    0.001172
     14          6           0        3.683503    0.442358    0.003107
     15          6           0        2.511844    1.156898    0.002098
     16          1           0        0.021842   -2.720827   -0.002860
     17          1           0       -4.587368   -1.559023    0.001906
     18          1           0       -2.421892   -2.756590   -0.001491
     19          1           0       -2.550400    2.220150    0.003681
     20          1           0       -4.626215    0.940944    0.005095
     21          1           0        4.606684   -1.532815    0.001702
     22          1           0        4.634652    0.968815    0.005593
     23          1           0        2.569768    2.238953    0.004553
     24          6           0       -0.062101    2.725091   -0.003719
     25          1           0       -0.575434    3.103335    0.889851
     26          1           0        0.922163    3.191489   -0.027576
     27          1           0       -0.614496    3.099147   -0.875073
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3942770      0.4478288
0.3396745
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9215151082 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860690272     A.U. after   10 cycles
             Convg  =    0.4460D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000021448    0.000001782    0.000000209
      2        6          -0.000017495   -0.000018435    0.000001069
      3        6           0.000006668    0.000015377    0.000004494
      4        6           0.000010717   -0.000001379   -0.000008476
      5        6           0.000002562    0.000013056    0.000011403
      6        6           0.000000760    0.000007259    0.000001064
      7        6          -0.000005286   -0.000012211   -0.000008744
```

```
      8        6          -0.000005539   -0.000013938   -0.000026150
      9        6           0.000029928    0.000001917   -0.000001610
     10        6          -0.000011530    0.000022151    0.000006122
     11        6           0.000018623    0.000001045   -0.000000540
     12        1          -0.000004444   -0.000000583    0.000002637
     13        6          -0.000010894   -0.000012352    0.000000515
     14        6          -0.000006403   -0.000003626   -0.000001666
     15        6           0.000002755   -0.000006539    0.000005622
     16        1          -0.000000211    0.000000336    0.000001795
     17        1          -0.000005794   -0.000001316    0.000000907
     18        1           0.000002801    0.000003144    0.000002033
     19        1           0.000002783    0.000024277    0.000004498
     20        1          -0.000000842   -0.000004211   -0.000001243
     21        1           0.000004430    0.000004892   -0.000001360
     22        1           0.000002481   -0.000000168   -0.000001015
     23        1          -0.000001796    0.000007174    0.000000554
     24        6          -0.000020615    0.000016106    0.000017068
     25        1          -0.000010956   -0.000012798    0.000004607
     26        1          -0.000007397   -0.000015909   -0.000000022
     27        1           0.000003246   -0.000015053   -0.000013769
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000029928 RMS     0.000010119


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000082348 RMS     0.000013465
 Search for a local minimum.
 Step number  48 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   37   38   39   40
41
                                                     42   43   44   45
46
                                                     47   48
 DE= -1.52D-06 DEPred=-1.45D-06 R= 1.04D+00
 SS=  1.41D+00  RLast= 6.57D-02 DXNew= 1.4142D-01 1.9712D-01
 Trust test= 1.04D+00 RLast= 6.57D-02 DXMaxT set to 1.41D-01
     Eigenvalues ---    0.00021   0.00979   0.01352   0.01574
0.01745
     Eigenvalues ---    0.01770   0.01813   0.01823   0.01910
0.01937
     Eigenvalues ---    0.01973   0.01980   0.02019   0.02061
0.02104
     Eigenvalues ---    0.02110   0.02145   0.02185   0.02211
0.02227
     Eigenvalues ---    0.02336   0.02350   0.05259   0.06539
0.10272
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.11700   0.14973   0.15514   0.15726
0.15953
     Eigenvalues ---    0.16000   0.16003   0.16003   0.16009
0.16077
     Eigenvalues ---    0.16359   0.19525   0.22000   0.22174
0.22452
     Eigenvalues ---    0.22674   0.23029   0.24138   0.24497
0.24982
     Eigenvalues ---    0.27238   0.28604   0.30035   0.31355
0.32694
     Eigenvalues ---    0.33569   0.33601   0.33631   0.33681
0.33682
     Eigenvalues ---    0.33766   0.34031   0.34173   0.35614
0.37027
     Eigenvalues ---    0.37407   0.37872   0.38157   0.39582
0.40307
     Eigenvalues ---    0.40886   0.41011   0.41987   0.44464
0.45631
     Eigenvalues ---    0.48925   0.49834   0.50921   0.51156
0.55628
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    48   47   46   45
44
 RFO step:  Lambda=-5.30821022D-08.
```

This journal is © The Royal Society of Chemistry 2014

```
 DIIS coeffs:      1.11281      0.02896      0.08678      0.00917
-0.23772
 Iteration  1 RMS(Cart)=  0.00388979 RMS(Int)=  0.00002372
 Iteration  2 RMS(Cart)=  0.00002458 RMS(Int)=  0.00000029
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000029
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59087   0.00000   0.00000  -0.00002  -0.00001
2.59085
    R2        2.69162   0.00001   0.00001   0.00002   0.00003
2.69165
    R3        2.05400   0.00000   0.00000   0.00001   0.00001
2.05401
    R4        2.70401   0.00001  -0.00002   0.00005   0.00003
2.70404
    R5        2.05593   0.00000   0.00001  -0.00002  -0.00001
2.05592
    R6        2.73036  -0.00002  -0.00008  -0.00001  -0.00008
2.73028
    R7        2.64305   0.00000   0.00003  -0.00003   0.00001
2.64305
    R8        2.71035  -0.00002  -0.00001  -0.00002  -0.00003
2.71032
    R9        2.68011  -0.00005   0.00003  -0.00009  -0.00005
2.68006
   R10        2.59576   0.00000   0.00000   0.00000   0.00000
2.59576
   R11        2.04949   0.00002   0.00001   0.00002   0.00003
2.04953
   R12        2.05442   0.00000   0.00001   0.00000   0.00000
2.05443
   R13        2.64081   0.00002  -0.00003   0.00005   0.00002
2.64083
   R14        2.05702   0.00000   0.00001  -0.00001  -0.00001
2.05702
   R15        2.67842   0.00002  -0.00008   0.00006  -0.00002
2.67841
   R16        2.86178   0.00000   0.00003  -0.00001   0.00003
2.86181
   R17        2.74099   0.00000   0.00007  -0.00006   0.00001
2.74100
   R18        2.71473   0.00000   0.00004  -0.00005  -0.00001
2.71472
   R19        2.70623   0.00001   0.00002   0.00002   0.00004
2.70627
   R20        2.05589   0.00000   0.00001  -0.00002  -0.00001
2.05589
   R21        2.58807  -0.00001  -0.00004   0.00000  -0.00004
2.58803
   R22        2.69245   0.00000   0.00004  -0.00001   0.00003
2.69249
```

This journal is © The Royal Society of Chemistry 2014

R23	2.05391	0.00000	0.00000	0.00001	0.00001
2.05393					
R24	2.59337	0.00000	-0.00004	0.00002	-0.00003
2.59334					
R25	2.05438	0.00000	0.00000	0.00000	0.00000
2.05438					
R26	2.04772	0.00001	0.00000	0.00002	0.00002
2.04775					
R27	2.07444	0.00001	-0.00016	0.00001	-0.00015
2.07429					
R28	2.05874	-0.00002	-0.00009	0.00004	-0.00005
2.05869					
R29	2.07381	0.00001	0.00019	0.00002	0.00021
2.07402					
A1	2.09060	0.00001	0.00001	0.00005	0.00005
2.09066					
A2	2.10173	0.00000	-0.00002	0.00004	0.00002
2.10175					
A3	2.09085	-0.00001	0.00001	-0.00008	-0.00007
2.09078					
A4	2.11524	-0.00001	-0.00001	-0.00004	-0.00005
2.11519					
A5	2.10419	0.00001	-0.00003	0.00008	0.00005
2.10424					
A6	2.06375	0.00000	0.00003	-0.00003	0.00000
2.06375					
A7	2.08416	-0.00001	0.00000	-0.00003	-0.00003
2.08413					
A8	2.11657	0.00002	0.00005	0.00004	0.00009
2.11665					
A9	2.08246	-0.00001	-0.00005	-0.00001	-0.00005
2.08240					
A10	2.04780	0.00003	0.00004	0.00008	0.00012
2.04792					
A11	2.09884	0.00002	0.00005	0.00001	0.00007
2.09891					
A12	2.13654	-0.00005	-0.00009	-0.00010	-0.00019
2.13636					
A13	2.12233	-0.00002	-0.00002	-0.00007	-0.00008
2.12225					
A14	2.08527	-0.00001	-0.00003	-0.00002	-0.00005
2.08522					
A15	2.07558	0.00002	0.00005	0.00008	0.00013
2.07572					
A16	2.10623	0.00000	-0.00002	0.00001	-0.00001
2.10623					
A17	2.08616	0.00000	0.00000	-0.00004	-0.00005
2.08611					
A18	2.09079	0.00001	0.00002	0.00003	0.00005
2.09084					
A19	2.11920	0.00000	0.00000	-0.00001	-0.00001
2.11918					

This journal is © The Royal Society of Chemistry 2014

A20	2.08261	0.00000	0.00000	0.00000	0.00000
2.08261					
A21	2.08138	0.00000	0.00000	0.00001	0.00001
2.08139					
A22	2.08829	0.00001	0.00002	0.00002	0.00004
2.08832					
A23	2.06729	-0.00008	-0.00038	-0.00002	-0.00040
2.06689					
A24	2.12761	0.00007	0.00036	0.00000	0.00036
2.12797					
A25	2.08728	-0.00002	-0.00006	-0.00003	-0.00010
2.08718					
A26	2.15726	0.00002	0.00013	-0.00006	0.00008
2.15734					
A27	2.03864	0.00000	-0.00007	0.00009	0.00002
2.03866					
A28	2.09031	0.00001	0.00004	0.00001	0.00006
2.09037					
A29	2.10646	-0.00001	-0.00006	0.00000	-0.00006
2.10640					
A30	2.08642	0.00000	0.00001	-0.00001	0.00000
2.08642					
A31	2.06106	0.00000	0.00000	-0.00003	-0.00003
2.06103					
A32	2.11770	-0.00001	0.00003	-0.00005	-0.00002
2.11768					
A33	2.10442	0.00001	-0.00002	0.00008	0.00006
2.10448					
A34	2.08775	0.00000	-0.00002	0.00003	0.00001
2.08776					
A35	2.10340	0.00000	0.00000	0.00005	0.00005
2.10345					
A36	2.09203	-0.00001	0.00002	-0.00008	-0.00006
2.09198					
A37	2.10860	0.00001	0.00001	0.00002	0.00003
2.10863					
A38	2.08615	-0.00001	-0.00001	-0.00004	-0.00005
2.08610					
A39	2.08844	0.00000	0.00000	0.00002	0.00002
2.08846					
A40	2.12726	-0.00001	0.00005	-0.00008	-0.00003
2.12723					
A41	2.09098	0.00001	0.00002	-0.00001	0.00001
2.09099					
A42	2.06495	0.00000	-0.00006	0.00008	0.00002
2.06497					
A43	1.94087	-0.00001	-0.00042	0.00009	-0.00033
1.94054					
A44	1.97405	0.00000	0.00030	-0.00014	0.00016
1.97421					
A45	1.94038	-0.00003	0.00002	-0.00012	-0.00010
1.94027					

This journal is © The Royal Society of Chemistry 2014

A46	1.86794	0.00001	-0.00032	0.00004	-0.00028	1.86767
A47	1.86868	0.00001	-0.00003	0.00008	0.00006	1.86874
A48	1.86655	0.00001	0.00046	0.00006	0.00052	1.86706
D1	-0.00006	0.00000	0.00006	-0.00004	0.00002	-0.00004
D2	3.14129	0.00000	0.00021	-0.00007	0.00014	3.14143
D3	-3.14144	0.00000	-0.00007	-0.00001	-0.00008	-3.14152
D4	-0.00010	0.00000	0.00009	-0.00004	0.00005	-0.00006
D5	0.00058	0.00000	-0.00025	-0.00005	-0.00029	0.00028
D6	-3.14092	0.00000	-0.00031	-0.00001	-0.00032	-3.14124
D7	-3.14122	0.00000	-0.00012	-0.00007	-0.00020	-3.14142
D8	0.00047	0.00000	-0.00019	-0.00004	-0.00023	0.00025
D9	-0.00076	0.00000	0.00035	0.00002	0.00037	-0.00039
D10	3.14072	0.00000	0.00046	-0.00007	0.00039	3.14111
D11	3.14108	0.00000	0.00020	0.00005	0.00025	3.14133
D12	-0.00063	0.00000	0.00030	-0.00004	0.00027	-0.00036
D13	0.00103	0.00000	-0.00055	0.00007	-0.00048	0.00055
D14	-3.14090	0.00000	-0.00027	-0.00005	-0.00033	-3.14123
D15	-3.14045	0.00001	-0.00066	0.00016	-0.00050	-3.14095
D16	0.00081	0.00000	-0.00038	0.00003	-0.00035	0.00046
D17	-3.14055	0.00001	-0.00066	0.00017	-0.00050	-3.14104
D18	0.00052	0.00000	-0.00020	-0.00006	-0.00027	0.00025
D19	0.00093	0.00000	-0.00056	0.00008	-0.00048	0.00046
D20	-3.14119	0.00000	-0.00010	-0.00015	-0.00025	-3.14144
D21	-0.00054	0.00000	0.00038	-0.00016	0.00022	-0.00032
D22	3.14014	0.00000	0.00080	-0.00007	0.00073	3.14087
D23	3.14140	0.00000	0.00009	-0.00003	0.00006	3.14146

This journal is © The Royal Society of Chemistry 2014

D24	-0.00111	0.00000	0.00051	0.00006	0.00057	-0.00053
D25	-0.00262	0.00000	0.00140	-0.00010	0.00130	-0.00132
D26	3.13981	0.00000	0.00071	0.00021	0.00092	3.14072
D27	3.13861	-0.00001	0.00170	-0.00024	0.00146	3.14007
D28	-0.00214	0.00000	0.00100	0.00008	0.00108	-0.00107
D29	-0.00026	0.00000	0.00002	0.00015	0.00017	-0.00009
D30	3.14123	0.00000	0.00008	0.00011	0.00020	3.14143
D31	-3.14095	0.00000	-0.00040	0.00006	-0.00034	-3.14129
D32	0.00054	0.00000	-0.00034	0.00003	-0.00031	0.00023
D33	-0.00083	0.00000	0.00046	-0.00012	0.00034	-0.00049
D34	3.14047	0.00000	0.00065	-0.00016	0.00049	3.14095
D35	3.14129	0.00000	-0.00001	0.00011	0.00011	3.14140
D36	-0.00060	0.00000	0.00019	0.00007	0.00026	-0.00034
D37	0.00271	0.00000	-0.00150	0.00007	-0.00143	0.00128
D38	-3.13823	0.00001	-0.00192	0.00023	-0.00169	-3.13991
D39	-3.13975	0.00000	-0.00078	-0.00026	-0.00104	-3.14078
D40	0.00250	0.00000	-0.00120	-0.00009	-0.00129	0.00121
D41	1.06197	-0.00001	-0.01266	-0.00059	-0.01325	1.04873
D42	-3.11877	0.00000	-0.01317	-0.00057	-0.01374	-3.13251
D43	-1.01849	-0.00001	-0.01236	-0.00067	-0.01303	-1.03152
D44	-2.07876	-0.00001	-0.01338	-0.00026	-0.01364	-2.09240
D45	0.02368	0.00000	-0.01388	-0.00025	-0.01413	0.00955
D46	2.12396	0.00000	-0.01307	-0.00035	-0.01342	2.11054
D47	-0.00101	0.00000	0.00058	0.00004	0.00063	-0.00038
D48	3.14087	0.00000	0.00039	0.00009	0.00048	3.14135
D49	3.13997	0.00000	0.00098	-0.00011	0.00087	3.14084

This journal is © The Royal Society of Chemistry 2014

```
   D50       -0.00133   0.00000   0.00079  -0.00007   0.00072  -
0.00061
   D51       -3.14144   0.00000  -0.00017   0.00001  -0.00016
3.14158
   D52        0.00132   0.00000  -0.00076  -0.00006  -0.00082
0.00049
   D53        0.00079   0.00000  -0.00058   0.00017  -0.00041
0.00038
   D54       -3.13964   0.00000  -0.00117   0.00010  -0.00107  -
3.14071
   D55        0.00087   0.00000  -0.00045  -0.00003  -0.00048
0.00039
   D56       -3.14037   0.00000  -0.00066   0.00000  -0.00066  -
3.14102
   D57       -3.14102   0.00000  -0.00026  -0.00008  -0.00033  -
3.14135
   D58        0.00093   0.00000  -0.00046  -0.00004  -0.00051
0.00043
   D59        0.00008   0.00000  -0.00011   0.00006  -0.00005
0.00003
   D60        3.14134   0.00000   0.00008   0.00004   0.00012
3.14146
   D61       -3.14115   0.00000  -0.00032   0.00009  -0.00023  -
3.14138
   D62        0.00011   0.00000  -0.00013   0.00007  -0.00006
0.00005
   D63       -0.00066   0.00000   0.00033   0.00004   0.00038  -
0.00028
   D64        3.14074   0.00000   0.00047  -0.00001   0.00046
3.14120
   D65        3.14127   0.00000   0.00014   0.00007   0.00021
3.14148
   D66       -0.00052   0.00000   0.00027   0.00002   0.00029  -
0.00023
   D67        0.00020   0.00000   0.00003  -0.00017  -0.00014
0.00006
   D68        3.14064   0.00000   0.00061  -0.00009   0.00052
3.14116
   D69       -3.14120   0.00000  -0.00010  -0.00011  -0.00022  -
3.14142
   D70       -0.00076   0.00000   0.00047  -0.00004   0.00043  -
0.00032
         Item               Value     Threshold  Converged?
 Maximum Force            0.000082     0.000450     YES
 RMS     Force            0.000013     0.000300     YES
 Maximum Displacement     0.030030     0.001800     NO
 RMS     Displacement     0.003890     0.001200     NO
 Predicted change in Energy=-2.467945D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
```

This journal is © The Royal Society of Chemistry 2014

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.793502	-5.417886	0.015804
2	6	0	-3.422742	-5.391573	0.011025
3	6	0	-2.705331	-4.153545	-0.000566
4	6	0	-3.438575	-2.908657	-0.007845
5	6	0	-4.870625	-2.987696	-0.002227
6	6	0	-5.524686	-4.195543	0.009219
7	6	0	-1.306994	-4.124654	-0.004881
8	6	0	-2.745743	-1.671237	-0.019808
9	6	0	-1.328430	-1.661152	-0.022969
10	6	0	-0.603294	-2.917337	-0.015540
11	6	0	0.828755	-2.906055	-0.019041
12	1	0	1.348545	-3.861761	-0.013546
13	6	0	1.531685	-1.730727	-0.028792
14	6	0	0.830109	-0.490644	-0.035596
15	6	0	-0.541864	-0.459092	-0.032827
16	1	0	-0.754365	-5.062452	0.000456
17	1	0	-5.325763	-6.365538	0.024687
18	1	0	-2.851623	-6.317547	0.016111
19	1	0	-5.455510	-2.074368	-0.006718
20	1	0	-6.611527	-4.221343	0.013380
21	1	0	2.618551	-1.737624	-0.031214
22	1	0	1.389637	0.441412	-0.042964
23	1	0	-1.033769	0.506432	-0.037828
24	6	0	-3.555691	-0.391656	-0.028261
25	1	0	-4.196819	-0.322148	0.859994
26	1	0	-2.937861	0.505437	-0.046336
27	1	0	-4.213998	-0.345062	-0.905198

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.371021	0.000000			
3	C	2.441164	1.430917	0.000000		
4	C	2.851774	2.483039	1.444800	0.000000	
5	C	2.431480	2.806272	2.459208	1.434240	0.000000
6	C	1.424358	2.418400	2.819684	2.451168	1.373616
7	C	3.718685	2.466116	1.398643	2.454037	3.740608
8	C	4.269891	3.781558	2.482712	1.418227	2.499699
9	C	5.110898	4.278240	2.847523	2.451369	3.782498
10	C	4.879710	3.751244	2.438646	2.835305	4.267931
11	C	6.157945	4.924829	3.747845	4.267346	5.699989
12	H	6.336176	5.010600	4.064385	4.881082	6.280302
13	C	7.321552	6.160335	4.880897	5.107978	6.524588
14	C	7.476988	6.489069	5.090915	4.906039	6.223724
15	C	6.532107	5.712333	4.281427	3.793669	5.013277
16	H	4.054775	2.688619	2.152297	3.441495	4.609578
17	H	1.086934	2.137822	3.429316	3.938599	3.408473

This journal is © The Royal Society of Chemistry 2014

18	H	2.140160	1.087948	2.169005	3.459136	3.894177
19	H	3.408500	3.890541	3.447680	2.182674	1.084564
20	H	2.176450	3.396733	3.906809	3.433834	2.133745
21	H	8.275570	7.060478	5.846481	6.169331	7.592843
22	H	8.518569	7.562117	6.155014	5.876719	7.138019
23	H	7.016838	6.363650	4.950849	4.176940	5.189572
24	C	5.176592	5.001838	3.856901	2.519806	2.910180
25	H	5.199542	5.197982	4.200560	2.831626	2.881421
26	H	6.207497	5.917189	4.665006	3.450830	3.992430
27	H	5.188218	5.189685	4.195114	2.824631	2.868803

		6	7	8	9	10
6	C	0.000000				
7	C	4.218312	0.000000			
8	C	3.754396	2.844201	0.000000		
9	C	4.902320	2.463662	1.417352	0.000000	
10	C	5.084734	1.397469	2.478482	1.450475	0.000000
11	C	6.483039	2.458985	3.781774	2.490632	1.432098
12	H	6.881369	2.668534	4.643450	3.465396	2.168321
13	C	7.474566	3.713429	4.277851	2.860967	2.442613
14	C	7.356066	4.215943	3.765735	2.455512	2.818490
15	C	6.228270	3.744669	2.515263	1.436569	2.459073
16	H	4.848461	1.088527	3.932726	3.449484	2.150487
17	H	2.179148	4.601406	5.356766	6.173507	5.847514
18	H	3.412949	2.682368	4.647656	4.899353	4.076446
19	H	2.122362	4.627511	2.739621	4.147746	4.924903
20	H	1.087155	5.305446	4.631245	5.870861	6.148181
21	H	8.506192	4.594400	5.364717	3.947730	3.431072
22	H	8.325379	5.303039	4.643833	3.436431	3.905601
23	H	6.502240	4.639256	2.770094	2.187571	3.450797
24	C	4.283445	4.358034	1.514402	2.563657	3.885341
25	H	4.182133	4.853674	2.167882	3.286367	4.518295
26	H	5.366000	4.909092	2.185296	2.699059	4.143251
27	H	4.168964	4.852480	2.167586	3.291949	4.521645

		11	12	13	14	15
11	C	0.000000				
12	H	1.087928	0.000000			
13	C	1.369526	2.138944	0.000000		
14	C	2.415468	3.410820	1.424802	0.000000	
15	C	2.804713	3.892579	2.432422	1.372338	0.000000
16	H	2.675201	2.421587	4.040702	4.838727	4.608382
17	H	7.060314	7.128587	8.277012	8.509569	7.600993
18	H	5.018436	4.865509	6.344630	6.892795	6.297530
19	H	6.339073	7.034912	6.995675	6.482131	5.172400
20	H	7.555715	7.968235	8.515682	8.324569	7.141252
21	H	2.137463	2.474911	1.086891	2.180253	3.409233
22	H	3.394214	4.303469	2.176824	1.087131	2.131127
23	H	3.887726	4.975653	3.403897	2.113813	1.083620
24	C	5.054271	6.007776	5.260656	4.386923	3.014585
25	H	5.718888	6.636490	5.965718	5.108862	3.764914
26	H	5.081970	6.119376	4.997757	3.897420	2.582886
27	H	5.724799	6.641092	5.975034	5.120588	3.776057

		16	17	18	19	20

```
   16  H    0.000000
   17  H    4.753557   0.000000
   18  H    2.444177   2.474621   0.000000
   19  H    5.570409   4.293245   4.978486   0.000000
   20  H    5.917261   2.500178   4.304760   2.438499   0.000000
   21  H    4.736248   9.194174   7.134475   8.081117   9.558514
   22  H    5.906872   9.562203   7.979680   7.292907   9.260835
   23  H    5.576020   8.102413   7.062167   5.119892   7.312036
   24  C    5.446520   6.230828   5.967735   2.537971   4.899629
   25  H    5.921130   6.204419   6.202137   2.325031   4.663828
   26  H    5.980905   7.274435   6.823815   3.604930   5.986805
   27  H    5.919716   6.192482   6.194793   2.310653   4.649460
                 21         22         23         24         25
   21  H    0.000000
   22  H    2.501712   0.000000
   23  H    4.286638   2.424283   0.000000
   24  C    6.319248   5.015026   2.677078   0.000000
   25  H    7.017627   5.710240   3.390799   1.097667   0.000000
   26  H    5.992100   4.327972   1.904111   1.089411   1.758211
   27  H    7.027575   5.723872   3.404590   1.097524   1.765424
                 26         27
   26  H    0.000000
   27  H    1.757703   0.000000
Stoichiometry    C15H12
Framework group  C1[X(C15H12)]
Deg. of freedom    75
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -3.651919   -1.005413    0.000666
     2          6           0       -2.452307   -1.669210   -0.000344
     3          6           0       -1.211236   -0.956982   -0.000618
     4          6           0       -1.222310    0.487776   -0.000302
     5          6           0       -2.501382    1.136633    0.000987
     6          6           0       -3.672506    0.418796    0.001510
     7          6           0        0.013534   -1.632363   -0.001074
     8          6           0       -0.002814    1.211791   -0.001016
     9          6           0        1.228953    0.510623   -0.000412
    10          6           0        1.227350   -0.939852   -0.000686
    11          6           0        2.472474   -1.647363   -0.000374
    12          1           0        2.443651   -2.734909   -0.000823
    13          6           0        3.669596   -0.982158    0.000676
    14          6           0        3.683521    0.442576    0.001513
    15          6           0        2.511853    1.157073    0.000953
    16          1           0        0.022104   -2.720856   -0.001458
    17          1           0       -4.587288   -1.559047    0.000931
    18          1           0       -2.421809   -2.756731   -0.000841
```

```
    19          1           0       -2.550132    2.220100    0.001946
    20          1           0       -4.626124    0.940829    0.002646
    21          1           0        4.606848   -1.532511    0.001029
    22          1           0        4.634668    0.969045    0.002716
    23          1           0        2.569724    2.239146    0.002043
    24          6           0       -0.062893    2.725001   -0.001808
    25          1           0       -0.588378    3.101582    0.885280
    26          1           0        0.921270    3.192064   -0.011427
    27          1           0       -0.603999    3.099717   -0.880074
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3943089      0.4478344
0.3396793
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9264687338 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 3.05D+03 ExpMxC= 4.57D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860690504     A.U. after    9 cycles
            Convg  =    0.5906D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000004407   -0.000000506   -0.000000864
      2        6          -0.000003698    0.000000113    0.000000170
      3        6           0.000004423   -0.000004720    0.000001865
      4        6           0.000006760    0.000006593   -0.000004320
      5        6          -0.000007755   -0.000007983   -0.000001072
      6        6          -0.000000743    0.000003536    0.000002255
      7        6          -0.000007878   -0.000004517   -0.000002483
      8        6          -0.000014191   -0.000001550    0.000003508
      9        6           0.000013058   -0.000003072    0.000005371
     10        6           0.000003886    0.000009376   -0.000000612
     11        6          -0.000005786   -0.000003851   -0.000000941
     12        1           0.000000557   -0.000000735    0.000000740
     13        6          -0.000001687    0.000007819   -0.000000495
     14        6           0.000009653   -0.000004139    0.000000784
     15        6          -0.000014698   -0.000000615   -0.000003879
     16        1           0.000001988   -0.000000296    0.000000831
     17        1          -0.000000425   -0.000000796    0.000000513
     18        1           0.000001449   -0.000000788    0.000001308
     19        1          -0.000000957   -0.000005691   -0.000000822
```

This journal is © The Royal Society of Chemistry 2014

```
     20        1           0.000000438   -0.000001166   -0.000000643
     21        1           0.000000449    0.000000345   -0.000001033
     22        1          -0.000000414    0.000000143   -0.000000279
     23        1          -0.000008018    0.000002092   -0.000001106
     24        6           0.000001862   -0.000003263    0.000007996
     25        1           0.000004652    0.000007497   -0.000007884
     26        1           0.000010412    0.000000490    0.000001394
     27        1           0.000002255    0.000005686   -0.000000300
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000014698 RMS     0.000004828


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000050206 RMS     0.000007437
 Search for a local minimum.
 Step number  49 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   37   38   39   40
41
                                                     42   43   44   45
46
                                                     47   48   49
 DE= -2.32D-07 DEPred=-2.47D-07 R= 9.41D-01
 Trust test= 9.41D-01 RLast= 3.35D-02 DXMaxT set to 1.41D-01
     Eigenvalues ---    0.00017   0.00984   0.01389   0.01592
0.01744
     Eigenvalues ---    0.01767   0.01810   0.01821   0.01900
0.01936
     Eigenvalues ---    0.01973   0.01980   0.02016   0.02063
0.02103
     Eigenvalues ---    0.02111   0.02145   0.02177   0.02213
0.02226
     Eigenvalues ---    0.02334   0.02346   0.05230   0.06472
0.10281
     Eigenvalues ---    0.11912   0.14608   0.15469   0.15722
0.15967
     Eigenvalues ---    0.16000   0.16002   0.16003   0.16013
0.16068
     Eigenvalues ---    0.16336   0.19418   0.21971   0.22021
0.22421
     Eigenvalues ---    0.22703   0.23028   0.24113   0.24500
0.25028
     Eigenvalues ---    0.27178   0.28689   0.30295   0.31029
0.32739
     Eigenvalues ---    0.33567   0.33598   0.33631   0.33675
0.33682
```

```
     Eigenvalues ---    0.33726   0.33933   0.34191   0.35688
0.37120
     Eigenvalues ---    0.37395   0.37942   0.38166   0.39654
0.40281
     Eigenvalues ---    0.40813   0.41019   0.42019   0.44562
0.45568
     Eigenvalues ---    0.49014   0.49838   0.50807   0.51092
0.56736
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    49   48   47   46
45
 RFO step:  Lambda=-1.32404382D-08.
 DIIS coeffs:      1.22259      0.03937     -0.07510     -0.14027
-0.04660
 Iteration  1 RMS(Cart)=  0.00198791 RMS(Int)=  0.00000558
 Iteration  2 RMS(Cart)=  0.00000579 RMS(Int)=  0.00000014
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000014
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59085   0.00000  -0.00001   0.00000  -0.00001
2.59085
    R2        2.69165   0.00000   0.00001   0.00000   0.00000
2.69165
```

This journal is © The Royal Society of Chemistry 2014

R3	2.05401	0.00000	0.00000	-0.00001	0.00000
2.05401					
R4	2.70404	0.00000	0.00001	-0.00001	0.00000
2.70404					
R5	2.05592	0.00000	0.00000	0.00001	0.00000
2.05593					
R6	2.73028	0.00001	0.00000	0.00002	0.00002
2.73030					
R7	2.64305	0.00000	0.00000	-0.00001	-0.00001
2.64305					
R8	2.71032	0.00001	-0.00003	0.00004	0.00002
2.71034					
R9	2.68006	0.00001	-0.00003	0.00003	0.00000
2.68006					
R10	2.59576	0.00000	0.00002	-0.00002	0.00000
2.59576					
R11	2.04953	0.00000	0.00002	-0.00003	-0.00001
2.04952					
R12	2.05443	0.00000	-0.00001	0.00000	0.00000
2.05442					
R13	2.64083	0.00000	0.00003	-0.00002	0.00001
2.64085					
R14	2.05702	0.00000	-0.00001	0.00001	0.00000
2.05702					
R15	2.67841	-0.00001	0.00006	-0.00003	0.00002
2.67843					
R16	2.86181	0.00000	-0.00010	0.00009	-0.00001
2.86179					
R17	2.74100	-0.00001	-0.00001	0.00000	-0.00001
2.74099					
R18	2.71472	-0.00001	-0.00002	0.00001	-0.00001
2.71472					
R19	2.70627	0.00000	0.00000	0.00000	-0.00001
2.70627					
R20	2.05589	0.00000	0.00000	0.00000	0.00000
2.05589					
R21	2.58803	0.00001	-0.00001	0.00002	0.00001
2.58803					
R22	2.69249	0.00000	0.00000	0.00000	-0.00001
2.69248					
R23	2.05393	0.00000	0.00001	-0.00001	0.00000
2.05392					
R24	2.59334	0.00001	0.00002	0.00000	0.00001
2.59336					
R25	2.05438	0.00000	-0.00001	0.00000	0.00000
2.05438					
R26	2.04775	0.00001	0.00001	-0.00001	0.00000
2.04774					
R27	2.07429	-0.00001	-0.00005	-0.00004	-0.00009
2.07420					
R28	2.05869	0.00001	0.00001	-0.00001	0.00000
2.05869					

This journal is © The Royal Society of Chemistry 2014

R29	2.07402	0.00000	0.00004	0.00005	0.00009
2.07411					
A1	2.09066	0.00000	0.00000	0.00000	0.00000
2.09065					
A2	2.10175	0.00000	0.00003	-0.00002	0.00001
2.10176					
A3	2.09078	0.00000	-0.00002	0.00002	0.00000
2.09077					
A4	2.11519	0.00000	-0.00002	0.00002	0.00000
2.11519					
A5	2.10424	0.00000	0.00006	-0.00005	0.00001
2.10425					
A6	2.06375	0.00000	-0.00004	0.00003	-0.00001
2.06374					
A7	2.08413	0.00000	0.00001	0.00000	0.00001
2.08414					
A8	2.11665	-0.00001	-0.00001	0.00000	-0.00002
2.11664					
A9	2.08240	0.00000	0.00000	0.00000	0.00000
2.08241					
A10	2.04792	-0.00001	0.00001	-0.00004	-0.00002
2.04790					
A11	2.09891	-0.00001	0.00000	-0.00001	0.00000
2.09890					
A12	2.13636	0.00002	-0.00002	0.00004	0.00003
2.13638					
A13	2.12225	0.00000	-0.00003	0.00003	0.00001
2.12225					
A14	2.08522	0.00000	0.00003	-0.00003	0.00001
2.08523					
A15	2.07572	-0.00001	-0.00001	-0.00001	-0.00001
2.07570					
A16	2.10623	0.00000	0.00002	-0.00001	0.00001
2.10623					
A17	2.08611	0.00000	-0.00001	0.00000	-0.00001
2.08610					
A18	2.09084	0.00000	-0.00001	0.00001	0.00000
2.09085					
A19	2.11918	0.00000	0.00000	0.00000	0.00000
2.11919					
A20	2.08261	0.00000	-0.00001	0.00002	0.00000
2.08262					
A21	2.08139	0.00000	0.00001	-0.00002	-0.00001
2.08138					
A22	2.08832	0.00000	0.00001	-0.00001	-0.00001
2.08832					
A23	2.06689	0.00005	0.00000	0.00006	0.00006
2.06695					
A24	2.12797	-0.00005	-0.00001	-0.00005	-0.00005
2.12792					
A25	2.08718	0.00001	-0.00001	0.00002	0.00001
2.08720					

```
   A26        2.15734  -0.00002   0.00000  -0.00001  -0.00001
2.15733
   A27        2.03866   0.00001   0.00001  -0.00001   0.00000
2.03866
   A28        2.09037   0.00000   0.00000   0.00000  -0.00001
2.09036
   A29        2.10640   0.00001  -0.00001   0.00001   0.00000
2.10640
   A30        2.08642   0.00000   0.00002  -0.00001   0.00001
2.08643
   A31        2.06103   0.00000  -0.00004   0.00004   0.00000
2.06103
   A32        2.11768   0.00000  -0.00002   0.00001  -0.00001
2.11767
   A33        2.10448   0.00000   0.00006  -0.00005   0.00001
2.10449
   A34        2.08776   0.00000   0.00000   0.00000   0.00000
2.08776
   A35        2.10345   0.00000   0.00003  -0.00002   0.00000
2.10346
   A36        2.09198   0.00000  -0.00003   0.00002   0.00000
2.09197
   A37        2.10863   0.00000   0.00002  -0.00002   0.00000
2.10863
   A38        2.08610   0.00000  -0.00001   0.00001   0.00000
2.08610
   A39        2.08846   0.00000  -0.00001   0.00001   0.00000
2.08846
   A40        2.12723   0.00000  -0.00003   0.00002  -0.00001
2.12722
   A41        2.09099   0.00000   0.00002  -0.00002   0.00000
2.09099
   A42        2.06497   0.00001   0.00001  -0.00001   0.00001
2.06497
   A43        1.94054   0.00001  -0.00005   0.00001  -0.00004
1.94050
   A44        1.97421  -0.00002   0.00000  -0.00005  -0.00005
1.97416
   A45        1.94027   0.00001   0.00013   0.00000   0.00013
1.94040
   A46        1.86767   0.00000  -0.00026   0.00002  -0.00024
1.86743
   A47        1.86874   0.00000   0.00001   0.00000   0.00001
1.86875
   A48        1.86706   0.00000   0.00016   0.00002   0.00019
1.86725
    D1       -0.00004   0.00000  -0.00002   0.00004   0.00002  -
0.00002
    D2        3.14143   0.00000   0.00008   0.00003   0.00011
3.14154
    D3       -3.14152   0.00000  -0.00006   0.00000  -0.00006  -
3.14158
```

This journal is © The Royal Society of Chemistry 2014

D4	-0.00006	0.00000	0.00003	0.00000	0.00003	-0.00003
D5	0.00028	0.00000	-0.00016	-0.00004	-0.00019	0.00009
D6	-3.14124	0.00000	-0.00017	-0.00009	-0.00025	-3.14149
D7	-3.14142	0.00000	-0.00011	-0.00001	-0.00011	-3.14153
D8	0.00025	0.00000	-0.00012	-0.00006	-0.00017	0.00007
D9	-0.00039	0.00000	0.00022	0.00005	0.00027	-0.00011
D10	3.14111	0.00000	0.00021	0.00013	0.00035	3.14146
D11	3.14133	0.00000	0.00013	0.00005	0.00018	3.14151
D12	-0.00036	0.00000	0.00013	0.00013	0.00026	-0.00010
D13	0.00055	0.00000	-0.00025	-0.00013	-0.00038	0.00017
D14	-3.14123	0.00000	-0.00021	-0.00004	-0.00025	-3.14147
D15	-3.14095	0.00000	-0.00025	-0.00021	-0.00045	-3.14140
D16	0.00046	0.00000	-0.00020	-0.00012	-0.00032	0.00014
D17	-3.14104	0.00000	-0.00024	-0.00017	-0.00041	-3.14145
D18	0.00025	0.00000	-0.00015	-0.00006	-0.00021	0.00004
D19	0.00046	0.00000	-0.00025	-0.00009	-0.00034	0.00012
D20	-3.14144	0.00000	-0.00016	0.00002	-0.00014	-3.14158
D21	-0.00032	0.00000	0.00009	0.00013	0.00022	-0.00010
D22	3.14087	0.00000	0.00038	0.00013	0.00051	3.14138
D23	3.14146	0.00000	0.00004	0.00004	0.00008	3.14154
D24	-0.00053	0.00000	0.00034	0.00004	0.00038	-0.00016
D25	-0.00132	0.00000	0.00070	0.00026	0.00097	-0.00036
D26	3.14072	0.00000	0.00059	0.00007	0.00067	3.14139
D27	3.14007	0.00000	0.00075	0.00036	0.00111	3.14118
D28	-0.00107	0.00000	0.00064	0.00017	0.00081	-0.00026
D29	-0.00009	0.00000	0.00012	-0.00005	0.00007	-0.00003

This journal is © The Royal Society of Chemistry 2014

D30	3.14143	0.00000	0.00013	0.00000	0.00013	3.14155
D31	-3.14129	0.00000	-0.00018	-0.00005	-0.00022	-3.14151
D32	0.00023	0.00000	-0.00017	0.00000	-0.00017	0.00007
D33	-0.00049	0.00000	0.00019	0.00015	0.00034	-0.00015
D34	3.14095	0.00000	0.00025	0.00020	0.00045	3.14140
D35	3.14140	0.00000	0.00010	0.00004	0.00014	3.14154
D36	-0.00034	0.00000	0.00016	0.00009	0.00025	-0.00009
D37	0.00128	0.00000	-0.00076	-0.00020	-0.00096	0.00032
D38	-3.13991	0.00000	-0.00094	-0.00032	-0.00126	-3.14117
D39	-3.14078	0.00000	-0.00065	0.00000	-0.00065	-3.14143
D40	0.00121	0.00000	-0.00083	-0.00012	-0.00095	0.00026
D41	1.04873	0.00000	-0.00401	-0.00222	-0.00623	1.04250
D42	-3.13251	0.00000	-0.00438	-0.00222	-0.00659	-3.13910
D43	-1.03152	-0.00001	-0.00408	-0.00222	-0.00630	-1.03782
D44	-2.09240	0.00000	-0.00412	-0.00241	-0.00653	-2.09893
D45	0.00955	0.00000	-0.00449	-0.00241	-0.00690	0.00265
D46	2.11054	-0.00001	-0.00419	-0.00241	-0.00660	2.10393
D47	-0.00038	0.00000	0.00032	-0.00001	0.00031	-0.00007
D48	3.14135	0.00000	0.00026	-0.00005	0.00021	3.14156
D49	3.14084	0.00000	0.00049	0.00010	0.00059	3.14143
D50	-0.00061	0.00000	0.00042	0.00006	0.00048	-0.00013
D51	3.14158	0.00000	-0.00006	0.00004	-0.00002	3.14156
D52	0.00049	0.00000	-0.00045	0.00006	-0.00039	0.00010
D53	0.00038	0.00000	-0.00023	-0.00008	-0.00031	0.00007
D54	-3.14071	0.00000	-0.00062	-0.00006	-0.00068	-3.14139
D55	0.00039	0.00000	-0.00025	-0.00005	-0.00030	0.00008

```
   D56       -3.14102   0.00000  -0.00038  -0.00005  -0.00043  -
3.14145
   D57       -3.14135   0.00000  -0.00019  -0.00001  -0.00020  -
3.14155
   D58        0.00043   0.00000  -0.00032  -0.00001  -0.00033
0.00010
   D59        0.00003   0.00000  -0.00001  -0.00002  -0.00003  -
0.00001
   D60        3.14146   0.00000   0.00010  -0.00001   0.00009
3.14154
   D61       -3.14138   0.00000  -0.00014  -0.00002  -0.00016  -
3.14154
   D62        0.00005   0.00000  -0.00003  -0.00001  -0.00004
0.00001
   D63       -0.00028   0.00000   0.00022   0.00000   0.00022  -
0.00006
   D64        3.14120   0.00000   0.00027   0.00004   0.00031
3.14151
   D65        3.14148   0.00000   0.00011  -0.00001   0.00010
3.14158
   D66       -0.00023   0.00000   0.00016   0.00003   0.00019  -
0.00004
   D67        0.00006   0.00000  -0.00009   0.00005  -0.00004
0.00002
   D68        3.14116   0.00000   0.00030   0.00003   0.00033
3.14149
   D69       -3.14142   0.00000  -0.00014   0.00001  -0.00013  -
3.14155
   D70       -0.00032   0.00000   0.00024  -0.00001   0.00024  -
0.00008
         Item               Value     Threshold  Converged?
 Maximum Force            0.000050     0.000450     YES
 RMS     Force            0.000007     0.000300     YES
 Maximum Displacement     0.015533     0.001800     NO
 RMS     Displacement     0.001988     0.001200     NO
 Predicted change in Energy=-3.522260D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793490   -5.417928    0.015716
      2          6           0       -3.422733   -5.391585    0.011576
      3          6           0       -2.705344   -4.153543    0.000065
      4          6           0       -3.438602   -2.908651   -0.007473
      5          6           0       -4.870660   -2.987736   -0.002672
      6          6           0       -5.524696   -4.195599    0.008512
      7          6           0       -1.307009   -4.124647   -0.004013
```

8	6	0	-2.745770	-1.671226	-0.019056
9	6	0	-1.328446	-1.661154	-0.022770
10	6	0	-0.603307	-2.917329	-0.015084
11	6	0	0.828738	-2.906055	-0.018889
12	1	0	1.348522	-3.861762	-0.013002
13	6	0	1.531665	-1.730731	-0.029551
14	6	0	0.830086	-0.490657	-0.037057
15	6	0	-0.541892	-0.459102	-0.033805
16	1	0	-0.754374	-5.062439	0.001650
17	1	0	-5.325739	-6.365587	0.024490
18	1	0	-2.851585	-6.317540	0.017037
19	1	0	-5.455578	-2.074436	-0.007864
20	1	0	-6.611536	-4.221431	0.011929
21	1	0	2.618529	-1.737623	-0.032278
22	1	0	1.389612	0.441389	-0.045441
23	1	0	-1.033806	0.506412	-0.039687
24	6	0	-3.555636	-0.391597	-0.026909
25	1	0	-4.201264	-0.325401	0.858273
26	1	0	-2.937654	0.505506	-0.038116
27	1	0	-4.209460	-0.341563	-0.907065

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.371016	0.000000			
3	C	2.441161	1.430918	0.000000		
4	C	2.851795	2.483058	1.444811	0.000000	
5	C	2.431487	2.806276	2.459208	1.434248	0.000000
6	C	1.424360	2.418396	2.819678	2.451180	1.373616
7	C	3.718671	2.466103	1.398640	2.454047	3.740612
8	C	4.269912	3.781572	2.482720	1.418228	2.499724
9	C	5.110906	4.278239	2.847520	2.451375	3.782525
10	C	4.879711	3.751242	2.438650	2.835318	4.267952
11	C	6.157934	4.924814	3.747842	4.267355	5.700006
12	H	6.336149	5.010572	4.064374	4.881086	6.280306
13	C	7.321548	6.160325	4.880896	5.107987	6.524611
14	C	7.476991	6.489062	5.090911	4.906044	6.223752
15	C	6.532113	5.712328	4.281421	3.793668	5.013302
16	H	4.054754	2.688601	2.152297	3.441507	4.609580
17	H	1.086933	2.137821	3.429316	3.938619	3.408476
18	H	2.140163	1.087949	2.168999	3.459149	3.894181
19	H	3.408497	3.890541	3.447685	2.182684	1.084561
20	H	2.176445	3.396723	3.906800	3.433844	2.133745
21	H	8.275565	7.060468	5.846481	6.169340	7.592866
22	H	8.518573	7.562109	6.155009	5.876721	7.138048
23	H	7.016844	6.363644	4.950838	4.176929	5.189594
24	C	5.176689	5.001902	3.856937	2.519848	2.910294
25	H	5.195620	5.195116	4.198686	2.829196	2.877038
26	H	6.207584	5.917216	4.664993	3.450849	3.992557
27	H	5.192504	5.192837	4.197194	2.827265	2.873559

		6	7	8	9	10
6	C	0.000000				

7	C	4.218302	0.000000			
8	C	3.754417	2.844211	0.000000		
9	C	4.902336	2.463658	1.417365	0.000000	
10	C	5.084742	1.397475	2.478495	1.450469	0.000000
11	C	6.483039	2.458984	3.781787	2.490630	1.432094
12	H	6.881354	2.668526	4.643459	3.465390	2.168316
13	C	7.474574	3.713429	4.277862	2.860966	2.442607
14	C	7.356081	4.215940	3.765743	2.455510	2.818481
15	C	6.228286	3.744665	2.515262	1.436565	2.459065
16	H	4.848447	1.088527	3.932737	3.449478	2.150489
17	H	2.179148	4.601393	5.356787	6.173514	5.847514
18	H	3.412950	2.682338	4.647659	4.899333	4.076423
19	H	2.122352	4.627527	2.739665	4.147799	4.924942
20	H	1.087153	5.305434	4.631269	5.870883	6.148189
21	H	8.506199	4.594402	5.364727	3.947728	3.431068
22	H	8.325396	5.303033	4.643837	3.436429	3.905589
23	H	6.502256	4.639248	2.770082	2.187565	3.450788
24	C	4.283560	4.358040	1.514396	2.563624	3.885320
25	H	4.177560	4.853300	2.167813	3.288397	4.519528
26	H	5.366130	4.909021	2.185256	2.698926	4.143128
27	H	4.173933	4.852984	2.167706	3.289914	4.520457

		11	12	13	14	15
11	C	0.000000				
12	H	1.087927	0.000000			
13	C	1.369528	2.138951	0.000000		
14	C	2.415467	3.410822	1.424798	0.000000	
15	C	2.804716	3.892582	2.432426	1.372345	0.000000
16	H	2.675193	2.421572	4.040697	4.838719	4.608376
17	H	7.060300	7.128555	8.277005	8.509570	7.600998
18	H	5.018396	4.865454	6.344594	6.892764	6.297505
19	H	6.339112	7.034937	6.995725	6.482190	5.172455
20	H	7.555716	7.968218	8.515694	8.324591	7.141275
21	H	2.137467	2.474926	1.086890	2.180246	3.409234
22	H	3.394210	4.303469	2.176817	1.087129	2.131132
23	H	3.887729	4.975655	3.403903	2.113823	1.083620
24	C	5.054236	6.007745	5.260601	4.386853	3.014508
25	H	5.721023	6.638154	5.969058	5.113063	3.768910
26	H	5.081814	6.119230	4.997564	3.897206	2.582666
27	H	5.722666	6.639451	5.971627	5.116265	3.771930

		16	17	18	19	20
16	H	0.000000				
17	H	4.753535	0.000000			
18	H	2.444138	2.474632	0.000000		
19	H	5.570420	4.293236	4.978486	0.000000	
20	H	5.917242	2.500167	4.304756	2.438487	0.000000
21	H	4.736246	9.194165	7.134439	8.081166	9.558523
22	H	5.906862	9.562204	7.979647	7.292970	9.260861
23	H	5.576011	8.102418	7.062143	5.119947	7.312061
24	C	5.446527	6.230928	5.967782	2.538128	4.899762
25	H	5.920675	6.200281	6.199600	2.320048	4.658837
26	H	5.980829	7.274530	6.823812	3.605130	5.986973
27	H	5.920309	6.196994	6.197587	2.316079	4.654879

This journal is © The Royal Society of Chemistry 2014

		21	22	23	24	25
21	H	0.000000				
22	H	2.501700	0.000000			
23	H	4.286642	2.424297	0.000000		
24	C	6.319188	5.014946	2.676978	0.000000	
25	H	7.021185	5.715117	3.395738	1.097618	0.000000
26	H	5.991898	4.327748	1.903849	1.089413	1.758018
27	H	7.023935	5.718830	3.399439	1.097571	1.765431

		26	27
26	H	0.000000	
27	H	1.757864	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.651933	-1.005408	0.000157
2	6	0	-2.452320	-1.669196	-0.000114
3	6	0	-1.211253	-0.956961	-0.000170
4	6	0	-1.222316	0.487808	-0.000081
5	6	0	-2.501406	1.136651	0.000281
6	6	0	-3.672524	0.418804	0.000411
7	6	0	0.013507	-1.632354	-0.000285
8	6	0	-0.002812	1.211810	-0.000280
9	6	0	1.228952	0.510612	-0.000126
10	6	0	1.227338	-0.939857	-0.000175
11	6	0	2.472445	-1.647388	-0.000063
12	1	0	2.443600	-2.734933	-0.000147
13	6	0	3.669578	-0.982195	0.000207
14	6	0	3.683519	0.442535	0.000376
15	6	0	2.511854	1.157050	0.000201
16	1	0	0.022069	-2.720848	-0.000367
17	1	0	-4.587302	-1.559040	0.000208
18	1	0	-2.421805	-2.756716	-0.000257
19	1	0	-2.550180	2.220114	0.000558
20	1	0	-4.626146	0.940825	0.000723
21	1	0	4.606825	-1.532555	0.000334
22	1	0	4.634673	0.968990	0.000667
23	1	0	2.569732	2.239123	0.000440
24	6	0	-0.062779	2.725018	-0.000444
25	1	0	-0.593880	3.100990	0.883492
26	1	0	0.921484	3.191965	-0.003088
27	1	0	-0.598172	3.100509	-0.881934

Rotational constants (GHZ): 1.3943001 0.4478337
0.3396783

```
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9253353874 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860690545     A.U. after    8 cycles
            Convg  =    0.5159D-08             -V/T =  2.0099
```

```
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000001935    0.000000928   -0.000000067
      2        6          -0.000001613    0.000000914    0.000000554
      3        6           0.000004138   -0.000000429   -0.000000942
      4        6           0.000004166    0.000002401   -0.000000885
      5        6          -0.000002668   -0.000006363   -0.000000108
      6        6           0.000001844    0.000003057   -0.000000027
      7        6          -0.000005280   -0.000000587    0.000001044
      8        6          -0.000006460   -0.000006118    0.000004982
      9        6           0.000006621   -0.000001695    0.000000156
     10        6           0.000000234    0.000003426   -0.000000782
     11        6          -0.000004151   -0.000001706   -0.000000010
     12        1           0.000001179   -0.000000277   -0.000000078
     13        6          -0.000002414    0.000005951    0.000000121
     14        6           0.000003941   -0.000003735   -0.000000409
     15        6          -0.000006783   -0.000001633    0.000000015
     16        1           0.000001505   -0.000000517   -0.000000284
     17        1          -0.000000386   -0.000001326    0.000000435
     18        1           0.000000573   -0.000000955    0.000000142
     19        1          -0.000000579   -0.000000535   -0.000000374
     20        1          -0.000001258   -0.000000315   -0.000000061
     21        1           0.000001199   -0.000000179   -0.000000602
     22        1           0.000000031    0.000001702    0.000000069
     23        1          -0.000004029    0.000002033    0.000000188
     24        6           0.000000386    0.000002135    0.000000807
     25        1           0.000004246    0.000001286   -0.000006012
     26        1           0.000004754   -0.000000108    0.000001491
     27        1          -0.000001129    0.000002643    0.000000637
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000006783 RMS     0.000002659


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000022612 RMS     0.000003410
 Search for a local minimum.
 Step number  50 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   37   38   39   40
41
                                                     42   43   44   45
46
```

This journal is © The Royal Society of Chemistry 2014

```
                                                     47   48   49   50
 DE= -4.12D-08 DEPred=-3.52D-08 R= 1.17D+00
 Trust test= 1.17D+00 RLast= 1.64D-02 DXMaxT set to 1.41D-01
     Eigenvalues ---    0.00015   0.01014   0.01426   0.01616
0.01741
     Eigenvalues ---    0.01763   0.01803   0.01818   0.01890
0.01938
     Eigenvalues ---    0.01973   0.01981   0.02012   0.02064
0.02102
     Eigenvalues ---    0.02111   0.02145   0.02171   0.02216
0.02226
     Eigenvalues ---    0.02327   0.02344   0.05272   0.06445
0.10338
     Eigenvalues ---    0.12098   0.14182   0.15427   0.15715
0.15962
     Eigenvalues ---    0.16000   0.16002   0.16002   0.16012
0.16085
     Eigenvalues ---    0.16250   0.19319   0.21870   0.22005
0.22402
     Eigenvalues ---    0.22721   0.23039   0.24017   0.24486
0.25029
     Eigenvalues ---    0.27110   0.28310   0.30076   0.31178
0.32734
     Eigenvalues ---    0.33554   0.33595   0.33630   0.33657
0.33682
     Eigenvalues ---    0.33696   0.33912   0.34187   0.35725
0.37110
     Eigenvalues ---    0.37305   0.37858   0.38175   0.39486
0.40296
     Eigenvalues ---    0.40828   0.40973   0.42131   0.44596
0.45609
     Eigenvalues ---    0.48964   0.49826   0.50817   0.51063
0.53797
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    50   49   48   47
46
 RFO step:  Lambda= 0.00000000D+00.
 DIIS coeffs:      1.43985     -0.41442     -0.06819      0.04027
0.00248
 Iteration  1 RMS(Cart)=  0.00072657 RMS(Int)=  0.00000076
 Iteration  2 RMS(Cart)=  0.00000079 RMS(Int)=  0.00000002
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59085   0.00000  -0.00001   0.00001   0.00000
2.59084
    R2        2.69165   0.00000   0.00000  -0.00001   0.00000
2.69165
    R3        2.05401   0.00000   0.00000   0.00001   0.00001
2.05401
    R4        2.70404   0.00000   0.00000   0.00000   0.00000
2.70405
    R5        2.05593   0.00000   0.00000   0.00000   0.00001
2.05593
    R6        2.73030   0.00000   0.00001   0.00000   0.00001
2.73031
    R7        2.64305   0.00000   0.00000  -0.00001  -0.00001
2.64303
    R8        2.71034   0.00000   0.00001  -0.00001   0.00000
2.71034
    R9        2.68006   0.00000   0.00000  -0.00002  -0.00002
2.68004
   R10        2.59576   0.00000   0.00000   0.00000  -0.00001
2.59575
   R11        2.04952   0.00000   0.00000   0.00001   0.00001
2.04953
   R12        2.05442   0.00000   0.00000   0.00001   0.00001
2.05443
   R13        2.64085   0.00000   0.00001   0.00000   0.00001
2.64085
   R14        2.05702   0.00000   0.00000   0.00000   0.00001
2.05702
   R15        2.67843  -0.00001   0.00001   0.00001   0.00001
2.67844
```

This journal is © The Royal Society of Chemistry 2014

R16	2.86179	0.00000	0.00000	0.00000	0.00000
2.86179					
R17	2.74099	-0.00001	-0.00001	-0.00001	-0.00002
2.74097					
R18	2.71472	-0.00001	-0.00001	-0.00001	-0.00001
2.71470					
R19	2.70627	0.00000	0.00000	-0.00001	-0.00001
2.70625					
R20	2.05589	0.00000	0.00000	0.00000	0.00000
2.05589					
R21	2.58803	0.00000	0.00000	0.00001	0.00001
2.58805					
R22	2.69248	0.00000	0.00000	-0.00002	-0.00002
2.69246					
R23	2.05392	0.00000	0.00000	0.00001	0.00001
2.05393					
R24	2.59336	0.00000	0.00000	0.00000	0.00001
2.59336					
R25	2.05438	0.00000	0.00000	0.00001	0.00001
2.05438					
R26	2.04774	0.00000	0.00000	0.00000	0.00001
2.04775					
R27	2.07420	-0.00001	-0.00004	-0.00002	-0.00005
2.07414					
R28	2.05869	0.00000	0.00000	0.00000	0.00000
2.05870					
R29	2.07411	0.00000	0.00003	0.00000	0.00003
2.07414					
A1	2.09065	0.00000	0.00000	0.00000	0.00000
2.09066					
A2	2.10176	0.00000	0.00000	-0.00001	-0.00001
2.10175					
A3	2.09077	0.00000	0.00000	0.00000	0.00000
2.09077					
A4	2.11519	0.00000	0.00000	0.00000	0.00000
2.11520					
A5	2.10425	0.00000	0.00000	-0.00001	0.00000
2.10424					
A6	2.06374	0.00000	0.00000	0.00000	0.00000
2.06374					
A7	2.08414	0.00000	0.00000	-0.00002	-0.00001
2.08413					
A8	2.11664	0.00000	-0.00001	0.00002	0.00001
2.11665					
A9	2.08241	0.00000	0.00000	0.00000	0.00000
2.08241					
A10	2.04790	0.00000	-0.00001	0.00001	0.00000
2.04790					
A11	2.09890	0.00000	-0.00001	0.00000	0.00000
2.09890					
A12	2.13638	0.00001	0.00002	-0.00002	0.00000
2.13638					

This journal is © The Royal Society of Chemistry 2014

A13	2.12225	0.00000	0.00000	0.00000	0.00000
2.12226					
A14	2.08523	0.00000	0.00000	-0.00001	-0.00001
2.08522					
A15	2.07570	0.00000	0.00000	0.00001	0.00000
2.07571					
A16	2.10623	0.00000	0.00000	-0.00001	-0.00001
2.10623					
A17	2.08610	0.00000	0.00000	0.00001	0.00001
2.08611					
A18	2.09085	0.00000	0.00000	0.00000	0.00000
2.09084					
A19	2.11919	0.00000	0.00000	0.00000	0.00000
2.11919					
A20	2.08262	0.00000	0.00000	0.00000	0.00001
2.08262					
A21	2.08138	0.00000	0.00000	0.00000	-0.00001
2.08138					
A22	2.08832	0.00000	0.00000	0.00000	0.00000
2.08832					
A23	2.06695	0.00002	0.00005	0.00001	0.00006
2.06701					
A24	2.12792	-0.00002	-0.00005	-0.00001	-0.00006
2.12785					
A25	2.08720	0.00000	0.00001	0.00000	0.00001
2.08720					
A26	2.15733	-0.00001	-0.00002	-0.00001	-0.00003
2.15730					
A27	2.03866	0.00001	0.00001	0.00001	0.00002
2.03868					
A28	2.09036	0.00000	0.00000	0.00000	-0.00001
2.09035					
A29	2.10640	0.00000	0.00000	0.00001	0.00002
2.10641					
A30	2.08643	0.00000	0.00000	-0.00001	-0.00001
2.08642					
A31	2.06103	0.00000	0.00000	0.00001	0.00001
2.06104					
A32	2.11767	0.00000	-0.00001	0.00000	0.00000
2.11767					
A33	2.10449	0.00000	0.00000	-0.00001	-0.00001
2.10448					
A34	2.08776	0.00000	0.00000	0.00001	0.00001
2.08776					
A35	2.10346	0.00000	0.00000	-0.00001	-0.00001
2.10344					
A36	2.09197	0.00000	0.00000	0.00001	0.00000
2.09198					
A37	2.10863	0.00000	0.00000	-0.00001	-0.00001
2.10862					
A38	2.08610	0.00000	0.00000	0.00001	0.00001
2.08611					

This journal is © The Royal Society of Chemistry 2014

A39	2.08846	0.00000	0.00000	0.00000	0.00000	2.08845
A40	2.12722	0.00000	-0.00001	0.00000	-0.00001	2.12722
A41	2.09099	0.00000	-0.00001	0.00001	0.00000	2.09099
A42	2.06497	0.00000	0.00001	-0.00001	0.00001	2.06498
A43	1.94050	0.00000	0.00001	-0.00003	-0.00002	1.94047
A44	1.97416	-0.00001	-0.00005	0.00001	-0.00004	1.97412
A45	1.94040	0.00001	0.00004	0.00004	0.00009	1.94049
A46	1.86743	0.00000	-0.00008	-0.00002	-0.00010	1.86733
A47	1.86875	0.00000	0.00001	-0.00004	-0.00002	1.86873
A48	1.86725	0.00000	0.00007	0.00003	0.00010	1.86735
D1	-0.00002	0.00000	0.00000	0.00001	0.00002	0.00000
D2	3.14154	0.00000	0.00003	0.00003	0.00006	-3.14159
D3	-3.14158	0.00000	-0.00002	0.00000	-0.00002	3.14158
D4	-0.00003	0.00000	0.00000	0.00001	0.00001	-0.00001
D5	0.00009	0.00000	-0.00006	-0.00003	-0.00009	0.00000
D6	-3.14149	0.00000	-0.00008	-0.00001	-0.00009	-3.14158
D7	-3.14153	0.00000	-0.00004	-0.00001	-0.00005	-3.14158
D8	0.00007	0.00000	-0.00006	0.00000	-0.00005	0.00002
D9	-0.00011	0.00000	0.00009	0.00003	0.00012	0.00000
D10	3.14146	0.00000	0.00012	0.00002	0.00013	3.14159
D11	3.14151	0.00000	0.00007	0.00001	0.00008	-3.14159
D12	-0.00010	0.00000	0.00009	0.00001	0.00010	0.00000
D13	0.00017	0.00000	-0.00012	-0.00005	-0.00017	0.00000
D14	-3.14147	0.00000	-0.00009	-0.00001	-0.00011	-3.14158
D15	-3.14140	0.00000	-0.00015	-0.00004	-0.00019	-3.14159
D16	0.00014	0.00000	-0.00012	0.00000	-0.00012	0.00002

This journal is © The Royal Society of Chemistry 2014

D17	-3.14145	0.00000	-0.00012	-0.00003	-0.00015	3.14158
D18	0.00004	0.00000	-0.00006	0.00003	-0.00004	0.00000
D19	0.00012	0.00000	-0.00010	-0.00004	-0.00013	-0.00002
D20	-3.14158	0.00000	-0.00004	0.00002	-0.00002	3.14159
D21	-0.00010	0.00000	0.00007	0.00003	0.00010	0.00000
D22	3.14138	0.00000	0.00017	0.00004	0.00021	3.14159
D23	3.14154	0.00000	0.00004	0.00000	0.00003	3.14158
D24	-0.00016	0.00000	0.00014	0.00001	0.00014	-0.00002
D25	-0.00036	0.00000	0.00032	0.00003	0.00035	-0.00001
D26	3.14139	0.00000	0.00021	-0.00004	0.00017	3.14157
D27	3.14118	0.00000	0.00035	0.00007	0.00042	-3.14158
D28	-0.00026	0.00000	0.00025	0.00000	0.00025	-0.00001
D29	-0.00003	0.00000	0.00002	0.00001	0.00003	0.00000
D30	3.14155	0.00000	0.00004	-0.00001	0.00003	3.14158
D31	-3.14151	0.00000	-0.00007	0.00000	-0.00008	-3.14159
D32	0.00007	0.00000	-0.00005	-0.00002	-0.00008	-0.00001
D33	-0.00015	0.00000	0.00011	0.00005	0.00016	0.00001
D34	3.14140	0.00000	0.00014	0.00005	0.00019	-3.14159
D35	3.14154	0.00000	0.00005	-0.00001	0.00004	3.14158
D36	-0.00009	0.00000	0.00008	-0.00001	0.00008	-0.00001
D37	0.00032	0.00000	-0.00031	-0.00002	-0.00033	0.00000
D38	-3.14117	0.00000	-0.00042	-0.00001	-0.00043	3.14159
D39	-3.14143	0.00000	-0.00020	0.00005	-0.00014	-3.14158
D40	0.00026	0.00000	-0.00031	0.00006	-0.00024	0.00002
D41	1.04250	0.00000	-0.00207	-0.00019	-0.00226	1.04024
D42	-3.13910	0.00000	-0.00221	-0.00023	-0.00244	-3.14154

This journal is © The Royal Society of Chemistry 2014

D43	-1.03782	0.00000	-0.00213	-0.00015	-0.00227	-1.04009
D44	-2.09893	0.00000	-0.00218	-0.00026	-0.00244	-2.10137
D45	0.00265	0.00000	-0.00232	-0.00030	-0.00262	0.00004
D46	2.10393	0.00000	-0.00224	-0.00022	-0.00245	2.10148
D47	-0.00007	0.00000	0.00010	-0.00002	0.00008	0.00000
D48	3.14156	0.00000	0.00006	-0.00002	0.00004	-3.14158
D49	3.14143	0.00000	0.00020	-0.00003	0.00017	-3.14159
D50	-0.00013	0.00000	0.00016	-0.00003	0.00014	0.00001
D51	3.14156	0.00000	0.00000	0.00003	0.00003	3.14159
D52	0.00010	0.00000	-0.00013	0.00001	-0.00011	-0.00001
D53	0.00007	0.00000	-0.00010	0.00003	-0.00007	0.00000
D54	-3.14139	0.00000	-0.00023	0.00002	-0.00021	3.14158
D55	0.00008	0.00000	-0.00011	0.00002	-0.00008	0.00000
D56	-3.14145	0.00000	-0.00015	0.00001	-0.00014	3.14159
D57	-3.14155	0.00000	-0.00007	0.00002	-0.00005	3.14159
D58	0.00010	0.00000	-0.00011	0.00000	-0.00011	-0.00001
D59	-0.00001	0.00000	-0.00001	0.00001	0.00000	0.00000
D60	3.14154	0.00000	0.00004	0.00001	0.00005	-3.14159
D61	-3.14154	0.00000	-0.00005	-0.00001	-0.00006	3.14158
D62	0.00001	0.00000	-0.00001	0.00000	-0.00001	0.00000
D63	-0.00006	0.00000	0.00007	0.00000	0.00007	0.00001
D64	3.14151	0.00000	0.00010	-0.00002	0.00008	-3.14159
D65	3.14158	0.00000	0.00003	-0.00001	0.00002	-3.14159
D66	-0.00004	0.00000	0.00006	-0.00002	0.00004	0.00000
D67	0.00002	0.00000	-0.00001	-0.00002	-0.00003	-0.00001
D68	3.14149	0.00000	0.00011	-0.00001	0.00011	-3.14159

```
   D69       -3.14155   0.00000  -0.00004  -0.00001  -0.00005
3.14159
   D70       -0.00008   0.00000   0.00008   0.00001   0.00009
0.00001
         Item               Value     Threshold  Converged?
 Maximum Force            0.000023     0.000450     YES
 RMS     Force            0.000003     0.000300     YES
 Maximum Displacement     0.005641     0.001800     NO
 RMS     Displacement     0.000727     0.001200     YES
 Predicted change in Energy=-5.118332D-09

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793497   -5.417941    0.015709
      2          6           0       -3.422740   -5.391600    0.011805
      3          6           0       -2.705342   -4.153562    0.000312
      4          6           0       -3.438608   -2.908671   -0.007314
      5          6           0       -4.870666   -2.987758   -0.002836
      6          6           0       -5.524706   -4.195616    0.008249
      7          6           0       -1.307013   -4.124664   -0.003685
      8          6           0       -2.745783   -1.671253   -0.018751
      9          6           0       -1.328453   -1.661182   -0.022666
     10          6           0       -0.603310   -2.917342   -0.014918
     11          6           0        0.828728   -2.906044   -0.018872
     12          1           0        1.348542   -3.861737   -0.012890
     13          6           0        1.531634   -1.730703   -0.029860
     14          6           0        0.830046   -0.490646   -0.037558
     15          6           0       -0.541937   -0.459117   -0.034089
     16          1           0       -0.754370   -5.062455    0.002061
     17          1           0       -5.325745   -6.365606    0.024449
     18          1           0       -2.851598   -6.317561    0.017408
     19          1           0       -5.455581   -2.074453   -0.008302
     20          1           0       -6.611551   -4.221443    0.011391
     21          1           0        2.618502   -1.737589   -0.032745
     22          1           0        1.389550    0.441413   -0.046281
     23          1           0       -1.033881    0.506384   -0.040231
     24          6           0       -3.555569   -0.391573   -0.026473
     25          1           0       -4.202866   -0.326535    0.857541
     26          1           0       -2.937485    0.505490   -0.035131
     27          1           0       -4.207731   -0.340251   -0.907805
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  C    1.371016   0.000000
    3  C    2.441165   1.430919   0.000000
```

This journal is © The Royal Society of Chemistry 2014

4	C	2.851788	2.483053	1.444815	0.000000	
5	C	2.431479	2.806271	2.459215	1.434248	0.000000
6	C	1.424360	2.418398	2.819689	2.451179	1.373613
7	C	3.718671	2.466104	1.398634	2.454048	3.740613
8	C	4.269894	3.781558	2.482711	1.418216	2.499713
9	C	5.110895	4.278229	2.847509	2.451370	3.782522
10	C	4.879714	3.751247	2.438649	2.835321	4.267954
11	C	6.157942	4.924826	3.747842	4.267352	5.700003
12	H	6.336185	5.010611	4.064396	4.881103	6.280326
13	C	7.321550	6.160335	4.880894	5.107976	6.524598
14	C	7.476985	6.489065	5.090909	4.906033	6.223736
15	C	6.532089	5.712313	4.281405	3.793643	5.013272
16	H	4.054764	2.688612	2.152297	3.441513	4.609587
17	H	1.086936	2.137820	3.429319	3.938616	3.408474
18	H	2.140161	1.087951	2.169003	3.459151	3.894179
19	H	3.408496	3.890541	3.447692	2.182682	1.084565
20	H	2.176453	3.396731	3.906814	3.433845	2.133743
21	H	8.275571	7.060480	5.846480	6.169332	7.592856
22	H	8.518566	7.562113	6.155007	5.876708	7.138026
23	H	7.016800	6.363613	4.950811	4.176888	5.189543
24	C	5.176739	5.001937	3.856964	2.519887	2.910364
25	H	5.194222	5.194107	4.198042	2.828337	2.875468
26	H	6.207609	5.917207	4.664966	3.450853	3.992620
27	H	5.194126	5.194037	4.197998	2.828288	2.875369

		6	7	8	9	10
6	C	0.000000				
7	C	4.218307	0.000000			
8	C	3.754404	2.844207	0.000000		
9	C	4.902331	2.463648	1.417372	0.000000	
10	C	5.084748	1.397480	2.478496	1.450458	0.000000
11	C	6.483044	2.458995	3.781777	2.490607	1.432088
12	H	6.881385	2.668555	4.643463	3.465377	2.168320
13	C	7.474570	3.713442	4.277845	2.860941	2.442606
14	C	7.356070	4.215952	3.765732	2.455502	2.818488
15	C	6.228258	3.744663	2.515243	1.436558	2.459066
16	H	4.848459	1.088530	3.932736	3.449469	2.150492
17	H	2.179152	4.601393	5.356772	6.173505	5.847517
18	H	3.412952	2.682346	4.647653	4.899330	4.076436
19	H	2.122354	4.627527	2.739650	4.147792	4.924940
20	H	1.087156	5.305443	4.631257	5.870879	6.148197
21	H	8.506199	4.594414	5.364713	3.947707	3.431065
22	H	8.325381	5.303049	4.643824	3.436424	3.905601
23	H	6.502205	4.639240	2.770050	2.187562	3.450788
24	C	4.283626	4.358039	1.514396	2.563586	3.885290
25	H	4.175925	4.853191	2.167774	3.289118	4.519985
26	H	5.366190	4.908947	2.185230	2.698816	4.143013
27	H	4.175814	4.853183	2.167781	3.289160	4.520011

		11	12	13	14	15
11	C	0.000000				
12	H	1.087930	0.000000			
13	C	1.369535	2.138953	0.000000		
14	C	2.415470	3.410821	1.424790	0.000000	

15	C	2.804712	3.892581	2.432416	1.372350	0.000000
16	H	2.675209	2.421608	4.040719	4.838737	4.608379
17	H	7.060310	7.128594	8.277012	8.509568	7.600977
18	H	5.018422	4.865507	6.344622	6.892782	6.297503
19	H	6.339100	7.034948	6.995699	6.482160	5.172414
20	H	7.555723	7.968253	8.515689	8.324578	7.141245
21	H	2.137468	2.474914	1.086893	2.180244	3.409233
22	H	3.394222	4.303475	2.176820	1.087132	2.131138
23	H	3.887729	4.975658	3.403900	2.113835	1.083623
24	C	5.054175	6.007706	5.260506	4.386748	3.014399
25	H	5.721792	6.638782	5.970231	5.114522	3.770275
26	H	5.081652	6.119084	4.997360	3.896996	2.582463
27	H	5.721837	6.638818	5.970298	5.114601	3.770352

		16	17	18	19	20
16	H	0.000000				
17	H	4.753543	0.000000			
18	H	2.444155	2.474623	0.000000		
19	H	5.570426	4.293242	4.978489	0.000000	
20	H	5.917260	2.500180	4.304764	2.438488	0.000000
21	H	4.736265	9.194175	7.134469	8.081143	9.558523
22	H	5.906886	9.562202	7.979669	7.292931	9.260841
23	H	5.576010	8.102378	7.062127	5.119880	7.312006
24	C	5.446529	6.230986	5.967816	2.538200	4.899833
25	H	5.920550	6.198812	6.198720	2.318231	4.657042
26	H	5.980751	7.274564	6.823793	3.605222	5.987055
27	H	5.920538	6.198706	6.198657	2.318122	4.656922

		21	22	23	24	25
21	H	0.000000				
22	H	2.501711	0.000000			
23	H	4.286650	2.424309	0.000000		
24	C	6.319094	5.014825	2.676832	0.000000	
25	H	7.022445	5.716796	3.397383	1.097589	0.000000
26	H	5.991694	4.327524	1.903611	1.089415	1.757930
27	H	7.022517	5.716886	3.397470	1.097586	1.765405

		26	27
26	H	0.000000	
27	H	1.757942	0.000000

Stoichiometry C15H12
Framework group C1[X(C15H12)]
Deg. of freedom 75
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.651950	-1.005368	-0.000013
2	6	0	-2.452347	-1.669174	-0.000009
3	6	0	-1.211265	-0.956962	0.000002
4	6	0	-1.222318	0.487811	0.000015

```
      5          6          0       -2.501399    1.136669    0.000013
      6          6          0       -3.672526    0.418843   -0.000003
      7          6          0        0.013482   -1.632366    0.000007
      8          6          0       -0.002815    1.211794    0.000012
      9          6          0        1.228947    0.510578    0.000004
     10          6          0        1.227324   -0.939880    0.000005
     11          6          0        2.472431   -1.647401    0.000007
     12          1          0        2.443605   -2.734949    0.000008
     13          6          0        3.669564   -0.982196    0.000000
     14          6          0        3.683506    0.442526   -0.000012
     15          6          0        2.511831    1.157034   -0.000005
     16          1          0        0.022038   -2.720863    0.000000
     17          1          0       -4.587326   -1.558995   -0.000033
     18          1          0       -2.421854   -2.756698   -0.000017
     19          1          0       -2.550152    2.220138    0.000023
     20          1          0       -4.626141    0.940884    0.000004
     21          1          0        4.606812   -1.532562   -0.000001
     22          1          0        4.634657    0.968994   -0.000021
     23          1          0        2.569693    2.239111   -0.000016
     24          6          0       -0.062670    2.725007   -0.000010
     25          1          0       -0.595815    3.100817    0.882727
     26          1          0        0.921652    3.191842   -0.000067
     27          1          0       -0.595935    3.100800   -0.882678
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3943061      0.4478347
0.3396792
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   309 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   309 basis functions,   528 primitive gaussians,   309 cartesian
basis functions
    51 alpha electrons       51 beta electrons
       nuclear repulsion energy       878.9262981312 Hartrees.
 NAtoms=   27 NActive=   27 NUniq=   27 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   309 RedAO= T  NBF=   309
 NBsUse=   302 1.00D-06 NBFU=   302
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -578.860690551     A.U. after    7 cycles
            Convg  =    0.9350D-08             -V/T =  2.0099
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000001457	-0.000003140	-0.000000886
2	6	-0.000000379	-0.000001611	0.000000072
3	6	-0.000000707	0.000000812	0.000001320
4	6	0.000001605	0.000000915	-0.000001123
5	6	-0.000003489	-0.000001165	0.000000126
6	6	-0.000001691	0.000003144	0.000001039
7	6	0.000000757	-0.000001652	-0.000001092
8	6	0.000001432	0.000000763	-0.000002448
9	6	-0.000002625	0.000001444	0.000000411
10	6	0.000000056	0.000000176	0.000001111
11	6	0.000001186	-0.000000870	-0.000000532
12	1	-0.000000282	0.000000886	0.000000207
13	6	0.000002162	-0.000001263	-0.000000268
14	6	-0.000000928	0.000002176	0.000000614
15	6	0.000001027	0.000001010	-0.000000794
16	1	0.000000110	0.000000966	0.000000194
17	1	0.000000430	0.000000914	0.000000481
18	1	-0.000000135	0.000000630	-0.000000052
19	1	0.000000757	-0.000001718	0.000000126

```
     20        1           0.000001377   -0.000001050   -0.000000454
     21        1          -0.000001132    0.000000369    0.000000021
     22        1          -0.000000598   -0.000001009   -0.000000018
     23        1           0.000000709   -0.000000996    0.000000367
     24        6           0.000000346    0.000001815    0.000004457
     25        1          -0.000000471   -0.000000395    0.000001185
     26        1          -0.000001351   -0.000001206   -0.000001400
     27        1           0.000000377    0.000000057   -0.000002663
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000004457 RMS     0.000001332


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000002918 RMS     0.000000759
 Search for a local minimum.
 Step number  51 out of a maximum of  157
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points   39   40   41   42
43
                                                     44   45   46   47
48
                                                     49   50   51
 DE= -5.21D-09 DEPred=-5.12D-09 R= 1.02D+00
 Trust test= 1.02D+00 RLast= 6.03D-03 DXMaxT set to 1.41D-01
     Eigenvalues ---    0.00013   0.00999   0.01466   0.01638
0.01739
     Eigenvalues ---    0.01756   0.01798   0.01817   0.01912
0.01939
     Eigenvalues ---    0.01973   0.01985   0.02020   0.02073
0.02105
     Eigenvalues ---    0.02114   0.02146   0.02169   0.02217
0.02226
     Eigenvalues ---    0.02321   0.02346   0.05293   0.06457
0.10379
     Eigenvalues ---    0.12076   0.14186   0.15514   0.15721
0.15936
     Eigenvalues ---    0.15990   0.16000   0.16003   0.16004
0.16086
     Eigenvalues ---    0.16263   0.19555   0.21857   0.22004
0.22447
     Eigenvalues ---    0.22770   0.23054   0.23911   0.24461
0.24972
     Eigenvalues ---    0.27254   0.27908   0.29973   0.31527
0.32660
     Eigenvalues ---    0.33547   0.33591   0.33628   0.33638
0.33682
```

```
     Eigenvalues ---    0.33690   0.33910   0.34187   0.35765
0.36942
     Eigenvalues ---    0.37190   0.37784   0.38178   0.39318
0.40283
     Eigenvalues ---    0.40799   0.40901   0.42259   0.44544
0.45935
     Eigenvalues ---    0.48825   0.49804   0.50932   0.51186
0.52632
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    51   50   49   48
47
 RFO step:  Lambda= 0.00000000D+00.
 DIIS coeffs:      0.66710      0.48913     -0.14601     -0.02241
0.01219
 Iteration  1 RMS(Cart)=  0.00001920 RMS(Int)=  0.00000000
 Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.59084   0.00000   0.00000   0.00000   0.00000
2.59084
    R2        2.69165   0.00000   0.00000   0.00000   0.00001
2.69165
```

This journal is © The Royal Society of Chemistry 2014

R3	2.05401	0.00000	0.00000	0.00000	0.00000
2.05401					
R4	2.70405	0.00000	0.00000	0.00000	0.00000
2.70405					
R5	2.05593	0.00000	0.00000	0.00000	0.00000
2.05593					
R6	2.73031	0.00000	0.00000	0.00000	0.00000
2.73031					
R7	2.64303	0.00000	0.00000	0.00000	0.00000
2.64304					
R8	2.71034	0.00000	0.00000	0.00000	0.00001
2.71034					
R9	2.68004	0.00000	0.00001	0.00000	0.00001
2.68005					
R10	2.59575	0.00000	0.00000	0.00000	0.00000
2.59575					
R11	2.04953	0.00000	0.00000	0.00000	0.00000
2.04953					
R12	2.05443	0.00000	0.00000	0.00000	0.00000
2.05442					
R13	2.64085	0.00000	0.00000	0.00000	0.00000
2.64085					
R14	2.05702	0.00000	0.00000	0.00000	0.00000
2.05702					
R15	2.67844	0.00000	0.00000	0.00000	0.00000
2.67844					
R16	2.86179	0.00000	0.00000	0.00000	0.00000
2.86180					
R17	2.74097	0.00000	0.00000	0.00000	0.00000
2.74097					
R18	2.71470	0.00000	0.00000	0.00000	0.00000
2.71471					
R19	2.70625	0.00000	0.00000	0.00000	0.00000
2.70626					
R20	2.05589	0.00000	0.00000	0.00000	0.00000
2.05589					
R21	2.58805	0.00000	0.00000	0.00000	0.00000
2.58804					
R22	2.69246	0.00000	0.00001	0.00000	0.00001
2.69247					
R23	2.05393	0.00000	0.00000	0.00000	0.00000
2.05393					
R24	2.59336	0.00000	0.00000	0.00000	0.00000
2.59336					
R25	2.05438	0.00000	0.00000	0.00000	0.00000
2.05438					
R26	2.04775	0.00000	0.00000	0.00000	0.00000
2.04775					
R27	2.07414	0.00000	0.00000	0.00000	0.00000
2.07415					
R28	2.05870	0.00000	0.00000	0.00000	0.00000
2.05869					

This journal is © The Royal Society of Chemistry 2014

R29	2.07414	0.00000	0.00000	0.00001	0.00001
2.07414					
A1	2.09066	0.00000	0.00000	0.00000	0.00000
2.09065					
A2	2.10175	0.00000	0.00000	0.00000	0.00001
2.10176					
A3	2.09077	0.00000	0.00000	0.00000	0.00000
2.09077					
A4	2.11520	0.00000	0.00000	0.00000	0.00000
2.11520					
A5	2.10424	0.00000	0.00000	0.00000	0.00000
2.10425					
A6	2.06374	0.00000	0.00000	0.00000	0.00000
2.06374					
A7	2.08413	0.00000	0.00001	0.00000	0.00001
2.08413					
A8	2.11665	0.00000	-0.00001	0.00000	-0.00001
2.11664					
A9	2.08241	0.00000	0.00000	0.00000	0.00000
2.08241					
A10	2.04790	0.00000	0.00000	0.00000	-0.00001
2.04790					
A11	2.09890	0.00000	0.00000	0.00000	0.00000
2.09890					
A12	2.13638	0.00000	0.00001	0.00000	0.00001
2.13639					
A13	2.12226	0.00000	0.00000	0.00000	0.00000
2.12226					
A14	2.08522	0.00000	0.00000	0.00000	0.00000
2.08522					
A15	2.07571	0.00000	0.00000	0.00000	0.00000
2.07571					
A16	2.10623	0.00000	0.00000	0.00000	0.00000
2.10623					
A17	2.08611	0.00000	0.00000	0.00000	-0.00001
2.08610					
A18	2.09084	0.00000	0.00000	0.00000	0.00001
2.09085					
A19	2.11919	0.00000	0.00000	0.00000	0.00000
2.11919					
A20	2.08262	0.00000	0.00000	0.00000	0.00000
2.08263					
A21	2.08138	0.00000	0.00000	0.00000	0.00000
2.08137					
A22	2.08832	0.00000	0.00000	0.00000	0.00000
2.08831					
A23	2.06701	0.00000	0.00000	0.00000	0.00000
2.06701					
A24	2.12785	0.00000	0.00000	0.00000	0.00000
2.12786					
A25	2.08720	0.00000	0.00000	0.00000	0.00000
2.08720					

This journal is © The Royal Society of Chemistry 2014

A26	2.15730	0.00000	0.00000	0.00000	0.00001
2.15731					
A27	2.03868	0.00000	0.00000	0.00000	-0.00001
2.03868					
A28	2.09035	0.00000	0.00000	0.00000	0.00000
2.09036					
A29	2.10641	0.00000	0.00000	0.00000	-0.00001
2.10641					
A30	2.08642	0.00000	0.00000	0.00000	0.00001
2.08642					
A31	2.06104	0.00000	0.00000	0.00000	0.00000
2.06104					
A32	2.11767	0.00000	0.00000	0.00000	0.00000
2.11767					
A33	2.10448	0.00000	0.00000	0.00000	0.00000
2.10448					
A34	2.08776	0.00000	0.00000	0.00000	0.00000
2.08776					
A35	2.10344	0.00000	0.00000	0.00000	0.00001
2.10345					
A36	2.09198	0.00000	0.00000	0.00000	0.00000
2.09197					
A37	2.10862	0.00000	0.00000	0.00000	0.00000
2.10862					
A38	2.08611	0.00000	0.00000	0.00000	-0.00001
2.08611					
A39	2.08845	0.00000	0.00000	0.00000	0.00000
2.08846					
A40	2.12722	0.00000	0.00000	0.00000	0.00000
2.12722					
A41	2.09099	0.00000	0.00000	0.00000	0.00000
2.09099					
A42	2.06498	0.00000	0.00000	0.00000	0.00000
2.06498					
A43	1.94047	0.00000	0.00001	-0.00001	0.00000
1.94048					
A44	1.97412	0.00000	0.00000	0.00000	0.00000
1.97411					
A45	1.94049	0.00000	-0.00001	0.00000	-0.00001
1.94048					
A46	1.86733	0.00000	0.00000	0.00001	0.00001
1.86734					
A47	1.86873	0.00000	0.00001	0.00001	0.00002
1.86874					
A48	1.86735	0.00000	-0.00001	-0.00001	-0.00001
1.86733					
D1	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D2	-3.14159	0.00000	-0.00001	0.00000	0.00000
3.14159					
D3	3.14158	0.00000	0.00000	0.00001	0.00001
3.14159					

This journal is © The Royal Society of Chemistry 2014

D4	-0.00001	0.00000	0.00000	0.00001	0.00001
0.00000					
D5	0.00000	0.00000	0.00001	0.00000	0.00001
0.00000					
D6	-3.14158	0.00000	0.00000	-0.00001	-0.00001
3.14159					
D7	-3.14158	0.00000	0.00000	-0.00001	-0.00001
3.14159					
D8	0.00002	0.00000	0.00000	-0.00001	-0.00002
0.00000					
D9	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D10	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D11	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D12	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D13	0.00000	0.00000	0.00001	0.00000	0.00001
0.00000					
D14	-3.14158	0.00000	0.00000	-0.00001	-0.00001
3.14159					
D15	-3.14159	0.00000	0.00001	0.00000	0.00000
3.14159					
D16	0.00002	0.00000	0.00000	-0.00001	-0.00001
0.00001					
D17	3.14158	0.00000	0.00000	0.00001	0.00001
3.14159					
D18	0.00000	0.00000	-0.00001	0.00000	-0.00001
0.00001					
D19	-0.00002	0.00000	0.00001	0.00001	0.00001
0.00000					
D20	3.14159	0.00000	-0.00001	0.00001	0.00000
3.14159					
D21	0.00000	0.00000	-0.00001	0.00001	0.00000
0.00000					
D22	3.14159	0.00000	-0.00001	0.00000	0.00000
3.14159					
D23	3.14158	0.00000	0.00000	0.00001	0.00001
3.14159					
D24	-0.00002	0.00000	0.00000	0.00001	0.00001
0.00001					
D25	-0.00001	0.00000	0.00001	0.00000	0.00000
0.00000					
D26	3.14157	0.00000	0.00002	0.00000	0.00003
3.14159					
D27	-3.14158	0.00000	-0.00001	0.00000	-0.00001
3.14159					
D28	-0.00001	0.00000	0.00001	0.00000	0.00001
0.00000					
D29	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					

This journal is © The Royal Society of Chemistry 2014

D30	3.14158	0.00000	0.00001	0.00000	0.00001
3.14159					
D31	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D32	-0.00001	0.00000	0.00000	0.00000	0.00001
0.00000					
D33	0.00001	0.00000	-0.00001	0.00000	-0.00001
0.00000					
D34	-3.14159	0.00000	-0.00001	0.00000	0.00000
3.14159					
D35	3.14158	0.00000	0.00000	0.00000	0.00001
3.14159					
D36	-0.00001	0.00000	0.00001	0.00001	0.00001
0.00000					
D37	0.00000	0.00000	-0.00001	0.00001	0.00000
0.00000					
D38	3.14159	0.00000	-0.00002	0.00002	0.00000
-3.14159					
D39	-3.14158	0.00000	-0.00003	0.00000	-0.00003
3.14158					
D40	0.00002	0.00000	-0.00004	0.00002	-0.00002
0.00000					
D41	1.04024	0.00000	-0.00004	-0.00002	-0.00006
1.04018					
D42	-3.14154	0.00000	-0.00003	-0.00002	-0.00005
-3.14159					
D43	-1.04009	0.00000	-0.00006	-0.00003	-0.00008
-1.04017					
D44	-2.10137	0.00000	-0.00002	-0.00002	-0.00004
-2.10141					
D45	0.00004	0.00000	-0.00002	-0.00001	-0.00003
0.00001					
D46	2.10148	0.00000	-0.00004	-0.00002	-0.00006
2.10142					
D47	0.00000	0.00000	0.00001	-0.00001	0.00000
0.00001					
D48	-3.14158	0.00000	0.00001	-0.00001	0.00000
-3.14159					
D49	-3.14159	0.00000	0.00002	-0.00002	0.00000
-3.14159					
D50	0.00001	0.00000	0.00002	-0.00002	-0.00001
0.00000					
D51	3.14159	0.00000	-0.00001	0.00001	0.00000
3.14159					
D52	-0.00001	0.00000	-0.00001	0.00001	0.00000
-0.00001					
D53	0.00000	0.00000	-0.00002	0.00002	0.00000
0.00000					
D54	3.14158	0.00000	-0.00002	0.00003	0.00001
3.14159					
D55	0.00000	0.00000	-0.00001	0.00001	0.00000
0.00000					

```
   D56        3.14159   0.00000  -0.00001   0.00001   0.00000
3.14159
   D57        3.14159   0.00000  -0.00001   0.00001   0.00000
3.14159
   D58       -0.00001   0.00000  -0.00001   0.00001   0.00001
0.00000
   D59        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D60       -3.14159   0.00000   0.00000   0.00000  -0.00001
3.14159
   D61        3.14158   0.00000   0.00000   0.00001   0.00001
3.14159
   D62        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D63        0.00001   0.00000   0.00000  -0.00001  -0.00001
0.00000
   D64       -3.14159   0.00000   0.00001  -0.00001   0.00000  -
3.14159
   D65       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D66        0.00000   0.00000   0.00001   0.00000   0.00001
0.00001
   D67       -0.00001   0.00000   0.00001   0.00000   0.00001
0.00000
   D68       -3.14159   0.00000   0.00001  -0.00001   0.00000  -
3.14159
   D69        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D70        0.00001   0.00000   0.00000  -0.00001  -0.00001
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.000003     0.000450     YES
 RMS     Force            0.000001     0.000300     YES
 Maximum Displacement     0.000112     0.001800     YES
 RMS     Displacement     0.000019     0.001200     YES
 Predicted change in Energy=-3.100052D-10
 Optimization completed.
    -- Stationary point found.
                           ----------------------------
                           !   Optimized Parameters   !
                           ! (Angstroms and Degrees)  !
 --------------------------                            ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ---------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.371          -DE/DX =    0.0
!
 ! R2    R(1,6)                  1.4244         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R3    R(1,17)                 1.0869          -DE/DX =    0.0
!
 ! R4    R(2,3)                  1.4309          -DE/DX =    0.0
!
 ! R5    R(2,18)                 1.088           -DE/DX =    0.0
!
 ! R6    R(3,4)                  1.4448          -DE/DX =    0.0
!
 ! R7    R(3,7)                  1.3986          -DE/DX =    0.0
!
 ! R8    R(4,5)                  1.4342          -DE/DX =    0.0
!
 ! R9    R(4,8)                  1.4182          -DE/DX =    0.0
!
 ! R10   R(5,6)                  1.3736          -DE/DX =    0.0
!
 ! R11   R(5,19)                 1.0846          -DE/DX =    0.0
!
 ! R12   R(6,20)                 1.0872          -DE/DX =    0.0
!
 ! R13   R(7,10)                 1.3975          -DE/DX =    0.0
!
 ! R14   R(7,16)                 1.0885          -DE/DX =    0.0
!
 ! R15   R(8,9)                  1.4174          -DE/DX =    0.0
!
 ! R16   R(8,24)                 1.5144          -DE/DX =    0.0
!
 ! R17   R(9,10)                 1.4505          -DE/DX =    0.0
!
 ! R18   R(9,15)                 1.4366          -DE/DX =    0.0
!
 ! R19   R(10,11)                1.4321          -DE/DX =    0.0
!
 ! R20   R(11,12)                1.0879          -DE/DX =    0.0
!
 ! R21   R(11,13)                1.3695          -DE/DX =    0.0
!
 ! R22   R(13,14)                1.4248          -DE/DX =    0.0
!
 ! R23   R(13,21)                1.0869          -DE/DX =    0.0
!
 ! R24   R(14,15)                1.3723          -DE/DX =    0.0
!
 ! R25   R(14,22)                1.0871          -DE/DX =    0.0
!
 ! R26   R(15,23)                1.0836          -DE/DX =    0.0
!
 ! R27   R(24,25)                1.0976          -DE/DX =    0.0
!
 ! R28   R(24,26)                1.0894          -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R29   R(24,27)              1.0976         -DE/DX =    0.0
!
 ! A1    A(2,1,6)             119.7859         -DE/DX =    0.0
!
 ! A2    A(2,1,17)            120.4216         -DE/DX =    0.0
!
 ! A3    A(6,1,17)            119.7926         -DE/DX =    0.0
!
 ! A4    A(1,2,3)             121.1919         -DE/DX =    0.0
!
 ! A5    A(1,2,18)            120.5642         -DE/DX =    0.0
!
 ! A6    A(3,2,18)            118.2438         -DE/DX =    0.0
!
 ! A7    A(2,3,4)             119.4116         -DE/DX =    0.0
!
 ! A8    A(2,3,7)             121.2749         -DE/DX =    0.0
!
 ! A9    A(4,3,7)             119.3135         -DE/DX =    0.0
!
 ! A10   A(3,4,5)             117.3363         -DE/DX =    0.0
!
 ! A11   A(3,4,8)             120.2581         -DE/DX =    0.0
!
 ! A12   A(5,4,8)             122.4057         -DE/DX =    0.0
!
 ! A13   A(4,5,6)             121.5964         -DE/DX =    0.0
!
 ! A14   A(4,5,19)            119.4743         -DE/DX =    0.0
!
 ! A15   A(6,5,19)            118.9293         -DE/DX =    0.0
!
 ! A16   A(1,6,5)             120.6779         -DE/DX =    0.0
!
 ! A17   A(1,6,20)            119.5255         -DE/DX =    0.0
!
 ! A18   A(5,6,20)            119.7966         -DE/DX =    0.0
!
 ! A19   A(3,7,10)            121.4205         -DE/DX =    0.0
!
 ! A20   A(3,7,16)            119.3255         -DE/DX =    0.0
!
 ! A21   A(10,7,16)           119.254          -DE/DX =    0.0
!
 ! A22   A(4,8,9)             119.6517         -DE/DX =    0.0
!
 ! A23   A(4,8,24)            118.4312         -DE/DX =    0.0
!
 ! A24   A(9,8,24)            121.9171         -DE/DX =    0.0
!
 ! A25   A(8,9,10)            119.5879         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A26   A(8,9,15)             123.6041         -DE/DX =    0.0
!
 ! A27   A(10,9,15)            116.808          -DE/DX =    0.0
!
 ! A28   A(7,10,9)             119.7685         -DE/DX =    0.0
!
 ! A29   A(7,10,11)            120.6886         -DE/DX =    0.0
!
 ! A30   A(9,10,11)            119.5429         -DE/DX =    0.0
!
 ! A31   A(10,11,12)           118.0888         -DE/DX =    0.0
!
 ! A32   A(10,11,13)           121.3335         -DE/DX =    0.0
!
 ! A33   A(12,11,13)           120.5777         -DE/DX =    0.0
!
 ! A34   A(11,13,14)           119.6201         -DE/DX =    0.0
!
 ! A35   A(11,13,21)           120.5185         -DE/DX =    0.0
!
 ! A36   A(14,13,21)           119.8614         -DE/DX =    0.0
!
 ! A37   A(13,14,15)           120.8149         -DE/DX =    0.0
!
 ! A38   A(13,14,22)           119.5255         -DE/DX =    0.0
!
 ! A39   A(15,14,22)           119.6596         -DE/DX =    0.0
!
 ! A40   A(9,15,14)            121.8805         -DE/DX =    0.0
!
 ! A41   A(9,15,23)            119.8048         -DE/DX =    0.0
!
 ! A42   A(14,15,23)           118.3147         -DE/DX =    0.0
!
 ! A43   A(8,24,25)            111.181          -DE/DX =    0.0
!
 ! A44   A(8,24,26)            113.1085         -DE/DX =    0.0
!
 ! A45   A(8,24,27)            111.1818         -DE/DX =    0.0
!
 ! A46   A(25,24,26)           106.9899         -DE/DX =    0.0
!
 ! A47   A(25,24,27)           107.0701         -DE/DX =    0.0
!
 ! A48   A(26,24,27)           106.9912         -DE/DX =    0.0
!
 ! D1    D(6,1,2,3)              0.0            -DE/DX =    0.0
!
 ! D2    D(6,1,2,18)           180.0            -DE/DX =    0.0
!
 ! D3    D(17,1,2,3)           179.9993         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D4    D(17,1,2,18)           -0.0006         -DE/DX =    0.0
!
 ! D5    D(2,1,6,5)             -0.0002         -DE/DX =    0.0
!
 ! D6    D(2,1,6,20)          -179.9995         -DE/DX =    0.0
!
 ! D7    D(17,1,6,5)          -179.9995         -DE/DX =    0.0
!
 ! D8    D(17,1,6,20)           0.0012          -DE/DX =    0.0
!
 ! D9    D(1,2,3,4)             0.0002          -DE/DX =    0.0
!
 ! D10   D(1,2,3,7)           179.9999          -DE/DX =    0.0
!
 ! D11   D(18,2,3,4)          180.0001          -DE/DX =    0.0
!
 ! D12   D(18,2,3,7)           -0.0002          -DE/DX =    0.0
!
 ! D13   D(2,3,4,5)            -0.0001          -DE/DX =    0.0
!
 ! D14   D(2,3,4,8)          -179.9993          -DE/DX =    0.0
!
 ! D15   D(7,3,4,5)          -179.9999          -DE/DX =    0.0
!
 ! D16   D(7,3,4,8)             0.0009          -DE/DX =    0.0
!
 ! D17   D(2,3,7,10)          179.9993          -DE/DX =    0.0
!
 ! D18   D(2,3,7,16)            0.0001          -DE/DX =    0.0
!
 ! D19   D(4,3,7,10)           -0.0009          -DE/DX =    0.0
!
 ! D20   D(4,3,7,16)          179.9999          -DE/DX =    0.0
!
 ! D21   D(3,4,5,6)            -0.0001          -DE/DX =    0.0
!
 ! D22   D(3,4,5,19)          179.9999          -DE/DX =    0.0
!
 ! D23   D(8,4,5,6)           179.9991          -DE/DX =    0.0
!
 ! D24   D(8,4,5,19)           -0.0009          -DE/DX =    0.0
!
 ! D25   D(3,4,8,9)            -0.0004          -DE/DX =    0.0
!
 ! D26   D(3,4,8,24)          -180.0015          -DE/DX =    0.0
!
 ! D27   D(5,4,8,9)           180.0005          -DE/DX =    0.0
!
 ! D28   D(5,4,8,24)           -0.0007          -DE/DX =    0.0
!
 ! D29   D(4,5,6,1)             0.0002          -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D30   D(4,5,6,20)           179.9995         -DE/DX =    0.0
!
 ! D31   D(19,5,6,1)          -179.9998         -DE/DX =    0.0
!
 ! D32   D(19,5,6,20)           -0.0005         -DE/DX =    0.0
!
 ! D33   D(3,7,10,9)            0.0003         -DE/DX =    0.0
!
 ! D34   D(3,7,10,11)          180.0001         -DE/DX =    0.0
!
 ! D35   D(16,7,10,9)          179.9995         -DE/DX =    0.0
!
 ! D36   D(16,7,10,11)          -0.0007         -DE/DX =    0.0
!
 ! D37   D(4,8,9,10)            -0.0002         -DE/DX =    0.0
!
 ! D38   D(4,8,9,15)          -180.0003         -DE/DX =    0.0
!
 ! D39   D(24,8,9,10)          180.001          -DE/DX =    0.0
!
 ! D40   D(24,8,9,15)            0.0009         -DE/DX =    0.0
!
 ! D41   D(4,8,24,25)           59.6016         -DE/DX =    0.0
!
 ! D42   D(4,8,24,26)         -179.9968         -DE/DX =    0.0
!
 ! D43   D(4,8,24,27)          -59.5929         -DE/DX =    0.0
!
 ! D44   D(9,8,24,25)         -120.3995         -DE/DX =    0.0
!
 ! D45   D(9,8,24,26)            0.002          -DE/DX =    0.0
!
 ! D46   D(9,8,24,27)          120.4059         -DE/DX =    0.0
!
 ! D47   D(8,9,10,7)             0.0003         -DE/DX =    0.0
!
 ! D48   D(8,9,10,11)         -179.9995         -DE/DX =    0.0
!
 ! D49   D(15,9,10,7)         -179.9997         -DE/DX =    0.0
!
 ! D50   D(15,9,10,11)           0.0005         -DE/DX =    0.0
!
 ! D51   D(8,9,15,14)          180.0            -DE/DX =    0.0
!
 ! D52   D(8,9,15,23)           -0.0006         -DE/DX =    0.0
!
 ! D53   D(10,9,15,14)          -0.0001         -DE/DX =    0.0
!
 ! D54   D(10,9,15,23)         179.9994         -DE/DX =    0.0
!
 ! D55   D(7,10,11,12)           0.0002         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D56   D(7,10,11,13)         179.9998         -DE/DX =    0.0
!
 ! D57   D(9,10,11,12)         179.9999         -DE/DX =    0.0
!
 ! D58   D(9,10,11,13)          -0.0004         -DE/DX =    0.0
!
 ! D59   D(10,11,13,14)         -0.0001         -DE/DX =    0.0
!
 ! D60   D(10,11,13,21)        180.0002         -DE/DX =    0.0
!
 ! D61   D(12,11,13,14)        179.9995         -DE/DX =    0.0
!
 ! D62   D(12,11,13,21)         -0.0002         -DE/DX =    0.0
!
 ! D63   D(11,13,14,15)          0.0005         -DE/DX =    0.0
!
 ! D64   D(11,13,14,22)       -179.9998         -DE/DX =    0.0
!
 ! D65   D(21,13,14,15)       -179.9997         -DE/DX =    0.0
!
 ! D66   D(21,13,14,22)          0.0            -DE/DX =    0.0
!
 ! D67   D(13,14,15,9)           -0.0004         -DE/DX =    0.0
!
 ! D68   D(13,14,15,23)       -179.9999         -DE/DX =    0.0
!
 ! D69   D(22,14,15,9)         179.9998         -DE/DX =    0.0
!
 ! D70   D(22,14,15,23)          0.0004         -DE/DX =    0.0
!
 ---------------------------------------------------------------------
-----------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -4.793497   -5.417941    0.015709
      2          6           0       -3.422740   -5.391600    0.011805
      3          6           0       -2.705342   -4.153562    0.000312
      4          6           0       -3.438608   -2.908671   -0.007314
      5          6           0       -4.870666   -2.987758   -0.002836
      6          6           0       -5.524706   -4.195616    0.008249
      7          6           0       -1.307013   -4.124664   -0.003685
      8          6           0       -2.745783   -1.671253   -0.018751
      9          6           0       -1.328453   -1.661182   -0.022666
     10          6           0       -0.603310   -2.917342   -0.014918
     11          6           0        0.828728   -2.906044   -0.018872
```

12	1	0	1.348542	-3.861737	-0.012890
13	6	0	1.531634	-1.730703	-0.029860
14	6	0	0.830046	-0.490646	-0.037558
15	6	0	-0.541937	-0.459117	-0.034089
16	1	0	-0.754370	-5.062455	0.002061
17	1	0	-5.325745	-6.365606	0.024449
18	1	0	-2.851598	-6.317561	0.017408
19	1	0	-5.455581	-2.074453	-0.008302
20	1	0	-6.611551	-4.221443	0.011391
21	1	0	2.618502	-1.737589	-0.032745
22	1	0	1.389550	0.441413	-0.046281
23	1	0	-1.033881	0.506384	-0.040231
24	6	0	-3.555569	-0.391573	-0.026473
25	1	0	-4.202866	-0.326535	0.857541
26	1	0	-2.937485	0.505490	-0.035131
27	1	0	-4.207731	-0.340251	-0.907805

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.371016	0.000000			
3	C	2.441165	1.430919	0.000000		
4	C	2.851788	2.483053	1.444815	0.000000	
5	C	2.431479	2.806271	2.459215	1.434248	0.000000
6	C	1.424360	2.418398	2.819689	2.451179	1.373613
7	C	3.718671	2.466104	1.398634	2.454048	3.740613
8	C	4.269894	3.781558	2.482711	1.418216	2.499713
9	C	5.110895	4.278229	2.847509	2.451370	3.782522
10	C	4.879714	3.751247	2.438649	2.835321	4.267954
11	C	6.157942	4.924826	3.747842	4.267352	5.700003
12	H	6.336185	5.010611	4.064396	4.881103	6.280326
13	C	7.321550	6.160335	4.880894	5.107976	6.524598
14	C	7.476985	6.489065	5.090909	4.906033	6.223736
15	C	6.532089	5.712313	4.281405	3.793643	5.013272
16	H	4.054764	2.688612	2.152297	3.441513	4.609587
17	H	1.086936	2.137820	3.429319	3.938616	3.408474
18	H	2.140161	1.087951	2.169003	3.459151	3.894179
19	H	3.408496	3.890541	3.447692	2.182682	1.084565
20	H	2.176453	3.396731	3.906814	3.433845	2.133743
21	H	8.275571	7.060480	5.846480	6.169332	7.592856
22	H	8.518566	7.562113	6.155007	5.876708	7.138026
23	H	7.016800	6.363613	4.950811	4.176888	5.189543
24	C	5.176739	5.001937	3.856964	2.519887	2.910364
25	H	5.194222	5.194107	4.198042	2.828337	2.875468
26	H	6.207609	5.917207	4.664966	3.450853	3.992620
27	H	5.194126	5.194037	4.197998	2.828288	2.875369

		6	7	8	9	10
6	C	0.000000				
7	C	4.218307	0.000000			
8	C	3.754404	2.844207	0.000000		
9	C	4.902331	2.463648	1.417372	0.000000	
10	C	5.084748	1.397480	2.478496	1.450458	0.000000

This journal is © The Royal Society of Chemistry 2014

11	C	6.483044	2.458995	3.781777	2.490607	1.432088
12	H	6.881385	2.668555	4.643463	3.465377	2.168320
13	C	7.474570	3.713442	4.277845	2.860941	2.442606
14	C	7.356070	4.215952	3.765732	2.455502	2.818488
15	C	6.228258	3.744663	2.515243	1.436558	2.459066
16	H	4.848459	1.088530	3.932736	3.449469	2.150492
17	H	2.179152	4.601393	5.356772	6.173505	5.847517
18	H	3.412952	2.682346	4.647653	4.899330	4.076436
19	H	2.122354	4.627527	2.739650	4.147792	4.924940
20	H	1.087156	5.305443	4.631257	5.870879	6.148197
21	H	8.506199	4.594414	5.364713	3.947707	3.431065
22	H	8.325381	5.303049	4.643824	3.436424	3.905601
23	H	6.502205	4.639240	2.770050	2.187562	3.450788
24	C	4.283626	4.358039	1.514396	2.563586	3.885290
25	H	4.175925	4.853191	2.167774	3.289118	4.519985
26	H	5.366190	4.908947	2.185230	2.698816	4.143013
27	H	4.175814	4.853183	2.167781	3.289160	4.520011

		11	12	13	14	15
11	C	0.000000				
12	H	1.087930	0.000000			
13	C	1.369535	2.138953	0.000000		
14	C	2.415470	3.410821	1.424790	0.000000	
15	C	2.804712	3.892581	2.432416	1.372350	0.000000
16	H	2.675209	2.421608	4.040719	4.838737	4.608379
17	H	7.060310	7.128594	8.277012	8.509568	7.600977
18	H	5.018422	4.865507	6.344622	6.892782	6.297503
19	H	6.339100	7.034948	6.995699	6.482160	5.172414
20	H	7.555723	7.968253	8.515689	8.324578	7.141245
21	H	2.137468	2.474914	1.086893	2.180244	3.409233
22	H	3.394222	4.303475	2.176820	1.087132	2.131138
23	H	3.887729	4.975658	3.403900	2.113835	1.083623
24	C	5.054175	6.007706	5.260506	4.386748	3.014399
25	H	5.721792	6.638782	5.970231	5.114522	3.770275
26	H	5.081652	6.119084	4.997360	3.896996	2.582463
27	H	5.721837	6.638818	5.970298	5.114601	3.770352

		16	17	18	19	20
16	H	0.000000				
17	H	4.753543	0.000000			
18	H	2.444155	2.474623	0.000000		
19	H	5.570426	4.293242	4.978489	0.000000	
20	H	5.917260	2.500180	4.304764	2.438488	0.000000
21	H	4.736265	9.194175	7.134469	8.081143	9.558523
22	H	5.906886	9.562202	7.979669	7.292931	9.260841
23	H	5.576010	8.102378	7.062127	5.119880	7.312006
24	C	5.446529	6.230986	5.967816	2.538200	4.899833
25	H	5.920550	6.198812	6.198720	2.318231	4.657042
26	H	5.980751	7.274564	6.823793	3.605222	5.987055
27	H	5.920538	6.198706	6.198657	2.318122	4.656922

		21	22	23	24	25
21	H	0.000000				
22	H	2.501711	0.000000			
23	H	4.286650	2.424309	0.000000		

This journal is © The Royal Society of Chemistry 2014

```
   24  C    6.319094   5.014825   2.676832   0.000000
   25  H    7.022445   5.716796   3.397383   1.097589   0.000000
   26  H    5.991694   4.327524   1.903611   1.089415   1.757930
   27  H    7.022517   5.716886   3.397470   1.097586   1.765405
                 26         27
   26  H    0.000000
   27  H    1.757942   0.000000
 Stoichiometry    C15H12
 Framework group  C1[X(C15H12)]
 Deg. of freedom    75
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.651950   -1.005368   -0.000013
      2          6           0       -2.452347   -1.669174   -0.000009
      3          6           0       -1.211265   -0.956962    0.000002
      4          6           0       -1.222318    0.487811    0.000015
      5          6           0       -2.501399    1.136669    0.000013
      6          6           0       -3.672526    0.418843   -0.000003
      7          6           0        0.013482   -1.632366    0.000007
      8          6           0       -0.002815    1.211794    0.000012
      9          6           0        1.228947    0.510578    0.000004
     10          6           0        1.227324   -0.939880    0.000005
     11          6           0        2.472431   -1.647401    0.000007
     12          1           0        2.443605   -2.734949    0.000008
     13          6           0        3.669564   -0.982196    0.000000
     14          6           0        3.683506    0.442526   -0.000012
     15          6           0        2.511831    1.157034   -0.000005
     16          1           0        0.022038   -2.720863    0.000000
     17          1           0       -4.587326   -1.558995   -0.000033
     18          1           0       -2.421854   -2.756698   -0.000017
     19          1           0       -2.550152    2.220138    0.000023
     20          1           0       -4.626141    0.940884    0.000004
     21          1           0        4.606812   -1.532562   -0.000001
     22          1           0        4.634657    0.968994   -0.000021
     23          1           0        2.569693    2.239111   -0.000016
     24          6           0       -0.062670    2.725007   -0.000010
     25          1           0       -0.595815    3.100817    0.882727
     26          1           0        0.921652    3.191842   -0.000067
     27          1           0       -0.595935    3.100800   -0.882678
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.3943061      0.4478347
0.3396792


*********************************************************************
```

This journal is © The Royal Society of Chemistry 2014

```
          Population analysis using the SCF density.

**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -10.20994 -10.20786 -10.20554 -10.20514 -
10.20445
 Alpha  occ. eigenvalues --  -10.19911 -10.19886 -10.19840 -10.19819 -
10.19810
 Alpha  occ. eigenvalues --  -10.19754 -10.19737 -10.19711 -10.19536 -
10.19046
 Alpha  occ. eigenvalues --   -0.88616  -0.85382  -0.80998  -0.79825
-0.75629
 Alpha  occ. eigenvalues --   -0.74319  -0.72844  -0.68674  -0.64692
-0.62177
 Alpha  occ. eigenvalues --   -0.59611  -0.58271  -0.54367  -0.52967
-0.50431
 Alpha  occ. eigenvalues --   -0.47066  -0.46792  -0.45616  -0.44261
-0.43742
 Alpha  occ. eigenvalues --   -0.43125  -0.41594  -0.41209  -0.39363
-0.39093
 Alpha  occ. eigenvalues --   -0.38406  -0.38361  -0.36550  -0.35218
-0.33817
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha  occ. eigenvalues --   -0.32764  -0.30763  -0.29421  -0.26181
-0.24581
 Alpha  occ. eigenvalues --   -0.19806
 Alpha virt. eigenvalues --   -0.07113  -0.02321  -0.00712   0.00363
0.01098
 Alpha virt. eigenvalues --    0.01282   0.02007   0.02637   0.02769
0.04548
 Alpha virt. eigenvalues --    0.04626   0.04833   0.04938   0.05635
0.06727
 Alpha virt. eigenvalues --    0.07017   0.07115   0.07280   0.07985
0.08993
 Alpha virt. eigenvalues --    0.09162   0.09356   0.10807   0.11212
0.11771
 Alpha virt. eigenvalues --    0.12386   0.12698   0.13128   0.13718
0.13815
 Alpha virt. eigenvalues --    0.14568   0.14707   0.15655   0.17178
0.17418
 Alpha virt. eigenvalues --    0.17844   0.18065   0.18164   0.18357
0.18523
 Alpha virt. eigenvalues --    0.19249   0.19481   0.19666   0.20088
0.20426
 Alpha virt. eigenvalues --    0.20718   0.21026   0.21949   0.22446
0.22825
 Alpha virt. eigenvalues --    0.23067   0.23351   0.24630   0.24691
0.24748
 Alpha virt. eigenvalues --    0.25270   0.25278   0.26086   0.26309
0.26862
 Alpha virt. eigenvalues --    0.27676   0.27805   0.27961   0.28863
0.29147
 Alpha virt. eigenvalues --    0.29368   0.30031   0.30634   0.31051
0.31723
 Alpha virt. eigenvalues --    0.31950   0.33761   0.34367   0.35774
0.35924
 Alpha virt. eigenvalues --    0.36778   0.37617   0.39118   0.39742
0.40232
 Alpha virt. eigenvalues --    0.42110   0.45928   0.48030   0.48938
0.51056
 Alpha virt. eigenvalues --    0.56712   0.58260   0.61445   0.64662
0.64765
 Alpha virt. eigenvalues --    0.64906   0.67289   0.67582   0.68091
0.70286
 Alpha virt. eigenvalues --    0.70598   0.70648   0.71704   0.72311
0.72362
 Alpha virt. eigenvalues --    0.73048   0.73623   0.74227   0.74397
0.74681
 Alpha virt. eigenvalues --    0.76146   0.77133   0.77674   0.77821
0.78382
 Alpha virt. eigenvalues --    0.79761   0.80090   0.80719   0.81040
0.81379
 Alpha virt. eigenvalues --    0.82980   0.86496   0.87917   0.89400
0.89992
```

```
 Alpha virt. eigenvalues --    0.90157   0.91579   0.92798   0.94362
0.94939
 Alpha virt. eigenvalues --    0.96969   0.98268   1.00715   1.01867
1.02778
 Alpha virt. eigenvalues --    1.04196   1.06956   1.08956   1.10302
1.10498
 Alpha virt. eigenvalues --    1.11471   1.12914   1.14366   1.17536
1.17985
 Alpha virt. eigenvalues --    1.18914   1.20061   1.20107   1.21166
1.22720
 Alpha virt. eigenvalues --    1.22832   1.23982   1.24046   1.26355
1.27384
 Alpha virt. eigenvalues --    1.32743   1.36196   1.36500   1.37454
1.37962
 Alpha virt. eigenvalues --    1.38977   1.40435   1.43995   1.44361
1.46459
 Alpha virt. eigenvalues --    1.48305   1.48836   1.49267   1.49584
1.49948
 Alpha virt. eigenvalues --    1.53604   1.55096   1.56015   1.57718
1.64077
 Alpha virt. eigenvalues --    1.75702   1.77817   1.78435   1.79555
1.81918
 Alpha virt. eigenvalues --    1.83315   1.86138   1.88574   1.90956
1.91733
 Alpha virt. eigenvalues --    1.92626   1.94489   1.95269   1.95493
1.96987
 Alpha virt. eigenvalues --    1.98955   2.00475   2.01685   2.03632
2.04787
 Alpha virt. eigenvalues --    2.06675   2.08189   2.13130   2.14666
2.16048
 Alpha virt. eigenvalues --    2.18710   2.20857   2.22404   2.24429
2.25181
 Alpha virt. eigenvalues --    2.26864   2.27720   2.28979   2.29547
2.30795
 Alpha virt. eigenvalues --    2.35593   2.37145   2.37463   2.39256
2.43250
 Alpha virt. eigenvalues --    2.44338   2.46928   2.50535   2.56335
2.57456
 Alpha virt. eigenvalues --    2.63214   2.65181   2.66046   2.67943
2.69241
 Alpha virt. eigenvalues --    2.70236   2.72766   2.74096   2.75617
2.82881
 Alpha virt. eigenvalues --    2.85900   2.86842   2.88921   2.93665
2.95102
 Alpha virt. eigenvalues --    2.95600   3.13236   3.13987   3.29654
3.43427
 Alpha virt. eigenvalues --    3.47829   4.20503   4.24137   4.25386
4.28487
 Alpha virt. eigenvalues --    4.30844   4.32346   4.33801   4.34392
4.40434
 Alpha virt. eigenvalues --    4.42471   4.43381   4.49687   4.52997
4.67958
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    4.86981
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C    6.060411   0.216370  -0.422654   0.094683  -0.820155
1.019949
     2  C    0.216370   7.019122  -0.280421  -0.742952   1.399804  -
0.964019
     3  C   -0.422654  -0.280421   7.677224  -0.015362   1.086784  -
0.506924
     4  C    0.094683  -0.742952  -0.015362   9.737940  -3.349132
1.022651
     5  C   -0.820155   1.399804   1.086784  -3.349132  11.848474  -
2.703275
     6  C    1.019949  -0.964019  -0.506924   1.022651  -2.703275
7.993494
     7  C    0.079087  -0.204917   0.585284  -1.058035   0.735102  -
0.430750
     8  C   -0.012466  -0.221769  -0.128448   1.433528  -1.278998
0.263721
     9  C   -0.011492  -0.040508  -0.717105  -0.061729  -0.355459
0.283803
    10  C    0.005287   0.029243  -0.955122  -0.793530  -0.196145
0.003513
    11  C   -0.039586  -0.256740   0.044012  -0.048697  -0.175166
0.047849
    12  H    0.000784   0.005083  -0.011589  -0.001472  -0.000047  -
0.000165
    13  C    0.020460  -0.047140  -0.024717  -0.053041  -0.066815
0.003823
    14  C    0.008884   0.053414   0.043968   0.184652   0.096190  -
0.044999
    15  C   -0.052934  -0.155083  -0.167923  -0.391408  -0.224923
0.090740
    16  H   -0.000542   0.005432  -0.053696   0.007706   0.002243
0.001314
    17  H    0.292878  -0.004504   0.001318   0.025267   0.003590  -
0.008069
    18  H    0.011619   0.264354  -0.037177   0.064643  -0.040643
0.016676
    19  H    0.015570  -0.030832   0.050083  -0.108425   0.263002
0.041681
    20  H   -0.017132   0.011897   0.008905  -0.009803   0.034408
0.271950
    21  H    0.000002   0.000058  -0.001797   0.000117  -0.000040  -
0.000005
    22  H    0.000001  -0.000009   0.000908  -0.001234  -0.000019
0.000012
    23  H    0.000081   0.000025   0.004505   0.015138   0.002637  -
0.000240
    24  C   -0.064683   0.051037  -0.223542  -0.409404   0.119862  -
0.063519
```

This journal is © The Royal Society of Chemistry 2014

25	H	0.001793	-0.000614	-0.014791	-0.048844	0.037710	0.032003
26	H	-0.000319	0.000317	-0.004128	0.021466	-0.029023	-0.009943
27	H	0.001793	-0.000613	-0.014796	-0.048838	0.037705	0.032003

		7	8	9	10	11	12
1	C	0.079087	-0.012466	-0.011492	0.005287	-0.039586	0.000784
2	C	-0.204917	-0.221769	-0.040508	0.029243	-0.256740	0.005083
3	C	0.585284	-0.128448	-0.717105	-0.955122	0.044012	-0.011589
4	C	-1.058035	1.433528	-0.061729	-0.793530	-0.048697	-0.001472
5	C	0.735102	-1.278998	-0.355459	-0.196145	-0.175166	-0.000047
6	C	-0.430750	0.263721	0.283803	0.003513	0.047849	-0.000165
7	C	6.929125	-0.361377	-1.025393	0.588896	-0.251256	-0.009126
8	C	-0.361377	6.953288	1.180165	-0.155132	-0.306482	0.003814
9	C	-1.025393	1.180165	9.080337	0.217719	-0.872256	0.069672
10	C	0.588896	-0.155132	0.217719	7.361291	-0.110800	-0.041197
11	C	-0.251256	-0.306482	-0.872256	-0.110800	7.019637	0.266340
12	H	-0.009126	0.003814	0.069672	-0.041197	0.266340	0.542971
13	C	-0.046986	-0.040611	0.346822	-0.523104	0.231585	0.019053
14	C	-0.338523	0.478515	1.238157	-0.508599	-0.962056	0.018491
15	C	0.631629	-1.253336	-3.340984	1.178274	1.467253	-0.042048
16	H	0.342790	-0.001660	0.008806	-0.051582	0.005209	0.004401
17	H	-0.013592	0.000772	0.000339	-0.002744	-0.000064	0.000000
18	H	-0.004424	0.004637	0.000016	-0.008503	0.005273	0.000002
19	H	0.006404	0.036382	0.009416	0.005885	0.000780	0.000000
20	H	0.002829	-0.005607	-0.001386	0.001104	0.000010	0.000000
21	H	-0.010616	0.000665	0.015817	0.006037	-0.006272	-0.004517
22	H	0.003425	-0.006406	-0.016666	0.011818	0.015017	-0.000169

This journal is © The Royal Society of Chemistry 2014

23	H	-0.000812	0.056801	-0.020408	-0.000200	-0.029275	0.000018
24	C	-0.067193	-0.567153	-0.301593	-0.263199	0.065335	-0.000350
25	H	-0.000275	-0.096119	-0.001112	-0.005567	-0.000552	0.000000
26	H	-0.000180	-0.091774	-0.013968	-0.025288	-0.003031	0.000000
27	H	-0.000276	-0.096119	-0.001108	-0.005564	-0.000553	0.000000

		13	14	15	16	17	18
1	C	0.020460	0.008884	-0.052934	-0.000542	0.292878	0.011619
2	C	-0.047140	0.053414	-0.155083	0.005432	-0.004504	0.264354
3	C	-0.024717	0.043968	-0.167923	-0.053696	0.001318	-0.037177
4	C	-0.053041	0.184652	-0.391408	0.007706	0.025267	0.064643
5	C	-0.066815	0.096190	-0.224923	0.002243	0.003590	-0.040643
6	C	0.003823	-0.044999	0.090740	0.001314	-0.008069	0.016676
7	C	-0.046986	-0.338523	0.631629	0.342790	-0.013592	-0.004424
8	C	-0.040611	0.478515	-1.253336	-0.001660	0.000772	0.004637
9	C	0.346822	1.238157	-3.340984	0.008806	0.000339	0.000016
10	C	-0.523104	-0.508599	1.178274	-0.051582	-0.002744	-0.008503
11	C	0.231585	-0.962056	1.467253	0.005209	-0.000064	0.005273
12	H	0.019053	0.018491	-0.042048	0.004401	0.000000	0.000002
13	C	6.148352	0.894552	-0.712096	-0.000152	-0.000005	0.000766
14	C	0.894552	7.208790	-2.339999	0.001775	-0.000001	-0.000120
15	C	-0.712096	-2.339999	11.344124	0.002065	0.000006	0.000104
16	H	-0.000152	0.001775	0.002065	0.539151	-0.000012	0.004339
17	H	-0.000005	-0.000001	0.000006	-0.000012	0.532747	-0.004502
18	H	0.000766	-0.000120	0.000104	0.004339	-0.004502	0.542531
19	H	0.000114	-0.000078	0.002236	0.000002	-0.000170	0.000017
20	H	0.000002	0.000003	-0.000089	0.000000	-0.003900	-0.000166

This journal is © The Royal Society of Chemistry 2014

21	H	0.292894	-0.016233	0.014259	-0.000013	0.000000	0.000000
22	H	-0.013699	0.275748	0.028109	0.000000	0.000000	0.000000
23	H	0.007237	0.044194	0.222240	0.000002	0.000000	0.000000
24	C	-0.045050	-0.037068	0.216763	0.001313	0.000462	-0.000267
25	H	-0.000703	0.002947	0.008171	0.000000	0.000000	0.000000
26	H	0.001876	-0.000021	-0.010073	0.000000	0.000000	0.000000
27	H	-0.000703	0.002945	0.008167	0.000000	0.000000	0.000000

		19	20	21	22	23	24
1	C	0.015570	-0.017132	0.000002	0.000001	0.000081	-0.064683
2	C	-0.030832	0.011897	0.000058	-0.000009	0.000025	0.051037
3	C	0.050083	0.008905	-0.001797	0.000908	0.004505	-0.223542
4	C	-0.108425	-0.009803	0.000117	-0.001234	0.015138	-0.409404
5	C	0.263002	0.034408	-0.000040	-0.000019	0.002637	0.119862
6	C	0.041681	0.271950	-0.000005	0.000012	-0.000240	-0.063519
7	C	0.006404	0.002829	-0.010616	0.003425	-0.000812	-0.067193
8	C	0.036382	-0.005607	0.000665	-0.006406	0.056801	-0.567153
9	C	0.009416	-0.001386	0.015817	-0.016666	-0.020408	-0.301593
10	C	0.005885	0.001104	0.006037	0.011818	-0.000200	-0.263199
11	C	0.000780	0.000010	-0.006272	0.015017	-0.029275	0.065335
12	H	0.000000	0.000000	-0.004517	-0.000169	0.000018	-0.000350
13	C	0.000114	0.000002	0.292894	-0.013699	0.007237	-0.045050
14	C	-0.000078	0.000003	-0.016233	0.275748	0.044194	-0.037068
15	C	0.002236	-0.000089	0.014259	0.028109	0.222240	0.216763
16	H	0.000002	0.000000	-0.000013	0.000000	0.000002	0.001313
17	H	-0.000170	-0.003900	0.000000	0.000000	0.000000	0.000462
18	H	0.000017	-0.000166	0.000000	0.000000	0.000000	-0.000267

This journal is © The Royal Society of Chemistry 2014

```
    19  H    0.544758  -0.004993   0.000000   0.000000  -0.000001  -
0.011778
    20  H   -0.004993   0.535187   0.000000   0.000000   0.000000  -
0.001449
    21  H    0.000000   0.000000   0.533079  -0.003825  -0.000182
0.000472
    22  H    0.000000   0.000000  -0.003825   0.535697  -0.005334  -
0.001357
    23  H   -0.000001   0.000000  -0.000182  -0.005334   0.554091  -
0.030528
    24  C   -0.011778  -0.001449   0.000472  -0.001357  -0.030528
7.241474
    25  H   -0.001086   0.000000   0.000000   0.000000  -0.000126
0.415279
    26  H    0.000200   0.000000   0.000000   0.000010   0.008589
0.497281
    27  H   -0.001086   0.000000   0.000000   0.000000  -0.000125
0.415283
             25         26         27
     1  C    0.001793  -0.000319   0.001793
     2  C   -0.000614   0.000317  -0.000613
     3  C   -0.014791  -0.004128  -0.014796
     4  C   -0.048844   0.021466  -0.048838
     5  C    0.037710  -0.029023   0.037705
     6  C    0.032003  -0.009943   0.032003
     7  C   -0.000275  -0.000180  -0.000276
     8  C   -0.096119  -0.091774  -0.096119
     9  C   -0.001112  -0.013968  -0.001108
    10  C   -0.005567  -0.025288  -0.005564
    11  C   -0.000552  -0.003031  -0.000553
    12  H    0.000000   0.000000   0.000000
    13  C   -0.000703   0.001876  -0.000703
    14  C    0.002947  -0.000021   0.002945
    15  C    0.008171  -0.010073   0.008167
    16  H    0.000000   0.000000   0.000000
    17  H    0.000000   0.000000   0.000000
    18  H    0.000000   0.000000   0.000000
    19  H   -0.001086   0.000200  -0.001086
    20  H    0.000000   0.000000   0.000000
    21  H    0.000000   0.000000   0.000000
    22  H    0.000000   0.000010   0.000000
    23  H   -0.000126   0.008589  -0.000125
    24  C    0.415279   0.497281   0.415283
    25  H    0.505337  -0.026341  -0.034664
    26  H   -0.026341   0.508731  -0.026339
    27  H   -0.034664  -0.026339   0.505337
 Mulliken atomic charges:
             1
     1  C   -0.387687
     2  C   -0.106033
     3  C    0.077202
     4  C    0.534117
```

This journal is © The Royal Society of Chemistry 2014

```
     5  C   -0.427672
     6  C   -0.393273
     7  C   -0.080841
     8  C    0.211170
     9  C    0.330097
    10  C    0.237208
    11  C   -0.105513
    12  H    0.180052
    13  C   -0.392713
    14  C   -0.305527
    15  C   -0.523243
    16  H    0.181112
    17  H    0.180182
    18  H    0.180825
    19  H    0.181919
    20  H    0.178230
    21  H    0.180102
    22  H    0.177974
    23  H    0.171674
    24  C   -0.936426
    25  H    0.227555
    26  H    0.201959
    27  H    0.227551
 Sum of Mulliken atomic charges =   0.00000
 Mulliken charges with hydrogens summed into heavy atoms:
               1
     1  C   -0.207505
     2  C    0.074792
     3  C    0.077202
     4  C    0.534117
     5  C   -0.245753
     6  C   -0.215043
     7  C    0.100271
     8  C    0.211170
     9  C    0.330097
    10  C    0.237208
    11  C    0.074539
    13  C   -0.212611
    14  C   -0.127553
    15  C   -0.351569
    24  C   -0.279361
 Sum of Mulliken charges with hydrogens summed into heavy atoms =
0.00000
 Electronic spatial extent (au):  <R**2>=           3169.5706
 Charge=              0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=             -0.0567    Y=              0.3423    Z=
0.0000  Tot=              0.3469
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=            -79.3230   YY=            -78.3703   ZZ=
-95.4863
```

XY= -0.0361 XZ= 0.0000 YZ=
0.0001
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= 5.0702 YY= 6.0229 ZZ=
-11.0931
XY= -0.0361 XZ= 0.0000 YZ=
0.0001
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= 0.2147 YYY= -3.7720 ZZZ=
0.0000 XYY= 0.0059
XXY= -1.3731 XXZ= -0.0007 XZZ=
-0.6370 YZZ= 3.9616
YYZ= -0.0001 XYZ= -0.0003
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -2923.3833 YYYY= -1099.6953 ZZZZ= -
125.3561 XXXY= 2.3443
XXXZ= 0.0002 YYYX= 1.5430 YYYZ=
0.0003 ZZZX= 0.0000
ZZZY= 0.0003 XXYY= -679.0438 XXZZ= -
631.2293 YYZZ= -229.9174
XXYZ= 0.0003 YYXZ= 0.0003 ZZXY=
-1.9180
N-N= 8.789262981312D+02 E-N=-3.096664609860D+03 KE=
5.731593383190D+02
1\1\GINC-OPT2620\FOpt\RB3LYP\6-31+G(d)\C15H12\UCN0868\17-Oct-
2012\0\\#
opt b3lyp/6-31+g(d) geom=connectivity\\methylanthracene\\0,1\C,-
4.793
4973716,-5.4179414809,0.0157085226\C,-3.4227401768,-
5.3915996983,0.011
8045204\C,-2.7053420978,-4.1535620694,0.000311612\C,-3.4386076482,-
2.9
08670547,-0.0073140638\C,-4.8706664514,-2.9877581948,-
0.0028360628\C,-
5.5247060688,-4.1956163048,0.0082487287\C,-1.3070127062,-
4.1246643502,
-0.0036849416\C,-2.7457831565,-1.6712534325,-0.018750881\C,-
1.32845283
03,-1.661182356,-0.022665798\C,-0.6033101091,-2.917342053,-
0.014918002
6\C,0.8287281045,-2.9060439119,-0.0188719762\H,1.3485420648,-
3.8617370
437,-0.0128904549\C,1.5316342024,-1.7307025133,-
0.0298603172\C,0.83004
56145,-0.490646219,-0.0375580793\C,-0.5419373478,-0.4591169937,-
0.0340
885051\H,-0.7543696748,-5.062454954,0.0020612048\H,-5.3257445835,-
6.36
56056341,0.0244488159\H,-2.8515978585,-6.3175605214,0.017408436\H,-
5.4
555805033,-2.0744526722,-0.0083021503\H,-6.6115511007,-
4.2214432074,0.

```
 0113913396\H,2.6185017818,-1.7375888826,-
0.0327447032\H,1.3895504353,0
 .441413442,-0.0462813521\H,-1.0338806318,0.5063844124,-
0.0402306453\C,
 -3.5555694936,-0.3915727255,-0.026472849\H,-4.2028656859,-
0.3265350612
 ,0.857540591\H,-2.9374849523,0.5054898273,-0.0351312857\H,-
4.207731084
 6,-0.3402508749,-0.907804793\\Version=AM64L-G09RevA.01\State=1-A\HF=-
5
 78.8606906\RMSD=9.350e-09\RMSF=1.332e-06\Dipole=-
0.0867679,0.1053678,-
 0.0005895\Quadrupole=3.9704928,4.2761344,-8.2466272,-0.3207189,-
0.0305
 423,-0.0958653\PG=C01 [X(C15H12)]\\@


 FORGIVE MY NONSENSE AS I ALSO FORGIVE THOSE WHO THINK THEY TALK SENSE

                                                        -- ROBERT FROST
 Job cpu time:  0 days 13 hours  1 minutes 34.9 seconds.
 File lengths (MBytes):  RWF=     64 Int=      0 D2E=      0 Chk=
7 Scr=      1
 Normal termination of Gaussian 09 at Wed Oct 17 00:15:50 2012.
```

This journal is © The Royal Society of Chemistry 2014

Transition State of Maleic Anhydride and 9-methylanthracene

```
Entering Gaussian System, Link 0=g09
 Initial command:
 /usr/local/g09a01/g09/l1.exe /tmp/pbstmp.8345804/Gau-20915.inp -
scrdir=/tmp/pbstmp.8345804/
 Entering Link 1 = /usr/local/g09a01/g09/l1.exe PID=     20916.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2009, Gaussian, Inc.
                    All Rights Reserved.

 This is part of the Gaussian(R) 09 program.  It is based on
 the Gaussian(R) 03 system (copyright 2003, Gaussian, Inc.),
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,
 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be
 used, copied, transmitted, or stored only in accord with that
 written license.

 The following legend is applicable only to US Government
 contracts under FAR:

                       RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is
 subject to restrictions as set forth in subparagraphs (a)
 and (c) of the Commercial Computer Software - Restricted
 Rights clause in FAR 52.227-19.

 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ----------------------------------------------------------------
 Warning -- This program may not be used in any manner that
 competes with the business of Gaussian, Inc. or will provide
 assistance to any competitor of Gaussian, Inc.  The licensee
 of this program is prohibited from giving any competitor of
 Gaussian, Inc. access to this program.  By using this program,
 the user acknowledges that Gaussian, Inc. is engaged in the
```

This journal is © The Royal Society of Chemistry 2014

```
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.
-----------------------------------------------------------------


Cite this work as:
Gaussian 09, Revision A.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

******************************************
Gaussian 09:  AM64L-G09RevA.01  8-May-2009
               18-Oct-2012
******************************************
%chk=daant.chk
%mem=450MW
%nprocshared=4
Will use up to    4 processors via shared memory.
--------------------------------------
# freq b3lyp/6-31+g(d) geom=connectivity
--------------------------------------
1/10=4,30=1,38=1,57=2/1,3;
2/12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,71=2,74=-5/1,2,3;
4//1;
5/5=2,38=5,98=1/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;
--------------------
methylanthracenefreq
--------------------
```

This journal is © The Royal Society of Chemistry 2014

```
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                     0.59649   0.18348  -1.33871
 C                    -0.41555   1.14999  -0.99321
 H                    -0.33798   2.13562  -1.44902
 C                     0.52643  -1.08094  -0.68765
 C                    -0.57473  -1.3104    0.22401
 C                     0.06126   0.39414   1.75001
 H                    -0.7393    0.07971   2.40434
 C                     0.10809   1.5846    0.99285
 H                    -0.60682   2.3938    1.07878
 C                     1.68392   0.48044  -2.18886
 H                     1.74029   1.46008  -2.65621
 C                     2.66085  -0.47056  -2.42682
 H                     3.48611  -0.2462   -3.09695
 C                     2.59528  -1.72693  -1.7892
 H                     3.36945  -2.46651  -1.97487
 C                     1.55983  -2.0224   -0.91932
 H                     1.53415  -2.98881  -0.42704
 C                    -1.81835  -0.61652  -0.05761
 C                    -1.73824   0.64807  -0.70441
 C                    -2.91024   1.39807  -0.93524
 H                    -2.83229   2.37054  -1.41642
 C                    -4.14852   0.89048  -0.57564
 H                    -5.05135   1.45955  -0.78044
 C                    -4.23752  -0.36836   0.05287
 H                    -5.21058  -0.76776   0.32622
 C                    -3.0931   -1.10195   0.32316
 H                    -3.18371  -2.06923   0.80679
 C                     1.54979   1.93596   0.85232
 C                     1.44209  -0.01627   2.02341
 O                     2.30228   0.8917    1.37516
 O                     1.88421  -0.93936   2.66176
 O                     2.06166   2.91329   0.37012
 C                    -0.58185  -2.55637   1.07271
 H                    -0.81315  -3.44321   0.46494
 H                     0.39113  -2.71382   1.54564
 H                    -1.32678  -2.49601   1.86993


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Initialization pass.
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
 Number of steps in this run=   2 maximum allowed number of steps=
2.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
```

This journal is © The Royal Society of Chemistry 2014

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.596488	0.183481	-1.338712
2	6	0	-0.415553	1.149994	-0.993208
3	1	0	-0.337978	2.135618	-1.449015
4	6	0	0.526431	-1.080941	-0.687648
5	6	0	-0.574729	-1.310401	0.224014
6	6	0	0.061263	0.394138	1.750010
7	1	0	-0.739299	0.079708	2.404342
8	6	0	0.108094	1.584598	0.992854
9	1	0	-0.606815	2.393798	1.078775
10	6	0	1.683917	0.480442	-2.188863
11	1	0	1.740288	1.460079	-2.656210
12	6	0	2.660852	-0.470562	-2.426819
13	1	0	3.486107	-0.246195	-3.096951
14	6	0	2.595277	-1.726925	-1.789198
15	1	0	3.369445	-2.466510	-1.974868
16	6	0	1.559833	-2.022403	-0.919320
17	1	0	1.534154	-2.988812	-0.427035
18	6	0	-1.818348	-0.616516	-0.057605
19	6	0	-1.738240	0.648072	-0.704407
20	6	0	-2.910235	1.398074	-0.935244
21	1	0	-2.832292	2.370537	-1.416424
22	6	0	-4.148519	0.890475	-0.575642
23	1	0	-5.051345	1.459548	-0.780441
24	6	0	-4.237524	-0.368363	0.052865
25	1	0	-5.210581	-0.767755	0.326218
26	6	0	-3.093103	-1.101954	0.323158
27	1	0	-3.183706	-2.069235	0.806786
28	6	0	1.549792	1.935964	0.852323
29	6	0	1.442090	-0.016267	2.023409
30	8	0	2.302277	0.891700	1.375159
31	8	0	1.884214	-0.939364	2.661757
32	8	0	2.061662	2.913290	0.370117
33	6	0	-0.581853	-2.556366	1.072706
34	1	0	-0.813150	-3.443208	0.464937
35	1	0	0.391125	-2.713821	1.545642
36	1	0	-1.326777	-2.496005	1.869933

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.441439	0.000000			
3	H	2.167079	1.088684	0.000000		
4	C	1.423923	2.440855	3.416597	0.000000	
5	C	2.458769	2.749638	3.837984	1.447872	0.000000
6	C	3.141822	2.885120	3.664138	2.886939	2.374574
7	H	3.975619	3.576824	4.385908	3.536889	2.591007
8	C	2.763667	2.099412	2.542701	3.178709	3.072195

This journal is © The Royal Society of Chemistry 2014

9	H	3.489654	2.424199	2.555123	4.059348	3.801675
10	C	1.411894	2.507123	2.715703	2.455878	3.759066
11	H	2.161893	2.740325	2.496570	3.435909	4.618501
12	C	2.423499	3.761078	4.091608	2.820112	4.266290
13	H	3.409681	4.647368	4.797119	3.906562	5.352731
14	C	2.801383	4.239736	4.861990	2.431220	3.778287
15	H	3.887986	5.326253	5.933051	3.414596	4.661349
16	C	2.443327	3.737875	4.601239	1.417019	2.523988
17	H	3.431299	4.609948	5.550595	2.173338	2.772781
18	C	2.848274	2.442078	3.420783	2.471970	1.451680
19	C	2.463563	1.443895	2.174389	2.849298	2.459947
20	C	3.732979	2.507657	2.724782	4.244702	3.759562
21	H	4.067651	2.740340	2.505564	4.870815	4.619192
22	C	4.857696	3.765202	4.102851	5.074858	4.272620
23	H	5.817047	4.650985	4.808315	6.129786	5.359257
24	C	5.060503	4.243482	4.871552	4.873540	3.785868
25	H	6.115463	5.330191	5.943340	5.834322	4.668622
26	C	4.245849	3.738096	4.605777	3.758084	2.528930
27	H	4.895688	4.611517	5.555861	4.120094	2.778887
28	C	2.963211	2.808258	2.983235	3.538431	3.930299
29	C	3.472578	3.729743	4.456117	3.053161	2.996692
30	O	3.282741	3.614205	4.061310	3.361564	3.801519
31	O	4.350031	4.797199	5.593934	3.616923	3.482335
32	O	3.538176	3.332336	3.110030	4.407911	4.981111
33	C	3.835386	4.246500	5.332285	2.550298	1.507567
34	H	4.288718	4.835470	5.917119	2.950125	2.159573
35	H	4.093413	4.693139	5.746009	2.769872	2.156192
36	H	4.601521	4.724533	5.783171	3.460926	2.163396

		6	7	8	9	10
6	C	0.000000				
7	H	1.080702	0.000000			
8	C	1.411621	2.230486	0.000000		
9	H	2.212583	2.670148	1.083181	0.000000	
10	C	4.260889	5.208656	3.718293	4.425589	0.000000
11	H	4.834266	5.801979	3.999404	4.508973	1.086867
12	C	4.995145	5.933291	4.736499	5.583135	1.383992
13	H	5.969306	6.944386	5.611531	6.415470	2.144881
14	C	4.842120	5.654122	4.989196	5.954748	2.421317
15	H	5.744745	6.522460	5.987926	6.982691	3.401665
16	C	3.900090	4.555393	4.332945	5.309386	2.809158
17	H	4.284073	4.754061	4.996580	5.985291	3.893866
18	C	2.796754	2.776735	3.107981	3.438192	4.243988
19	C	3.053990	3.314399	2.677074	2.739967	3.734015
20	C	4.128956	4.195699	3.586455	3.217683	4.849726
21	H	4.722829	4.922070	3.881777	3.343547	4.956336
22	C	4.835005	4.600047	4.589198	4.188167	6.065305
23	H	5.803192	5.535390	5.457108	4.907479	6.950256
24	C	4.684152	4.238843	4.856133	4.675903	6.388214
25	H	5.582967	5.002915	5.853740	5.635284	7.444309
26	C	3.771501	3.356791	4.232460	4.355785	5.624424
27	H	4.181830	3.625640	4.921490	5.160718	6.258476
28	C	2.323529	3.330824	1.490537	2.216269	3.374218

This journal is © The Royal Society of Chemistry 2014

29	C	1.466241	2.216479	2.324727	3.301327	4.248345
30	O	2.325989	3.312059	2.332532	3.287394	3.640571
31	O	2.435705	2.826233	3.508593	4.452081	5.058111
32	O	3.500261	4.473549	2.443287	2.809419	3.551031
33	C	3.094804	2.957521	4.198808	4.950231	4.999375
34	H	4.140197	4.022149	5.138698	5.872820	5.354720
35	H	3.132089	3.133533	4.343050	5.225095	5.081452
36	H	3.208421	2.695370	4.413552	5.005442	5.864925
		11	12	13	14	15
11	H	0.000000				
12	C	2.151147	0.000000			
13	H	2.480626	1.086491	0.000000		
14	C	3.411702	1.410429	2.167108	0.000000	
15	H	4.305401	2.165681	2.490478	1.086644	0.000000
16	C	3.895771	2.427552	3.406982	1.384247	2.141520
17	H	4.980396	3.407370	4.296571	2.138651	2.457006
18	C	4.871230	5.069291	6.124704	4.869446	5.831944
19	C	4.070509	4.854900	5.815306	5.059323	6.115811
20	C	4.959126	6.062475	6.949085	6.387920	7.446490
21	H	4.824364	6.266368	7.042274	6.810775	7.884822
22	C	6.271464	7.186572	8.120131	7.335004	8.351465
23	H	7.045906	8.118736	9.009099	8.345180	9.367513
24	C	6.812967	7.331226	8.342107	7.205974	8.147386
25	H	7.884967	8.344279	9.360689	8.144103	9.044203
26	C	6.229150	6.408512	7.464280	6.100025	6.993387
27	H	6.978117	6.868101	7.940343	6.344522	7.130162
28	C	3.545780	4.216467	4.909980	4.635453	5.539488
29	C	4.916030	4.636410	5.518058	4.334993	5.069971
30	O	4.109845	4.054549	4.764035	4.117791	4.862006
31	O	5.835993	5.168805	6.017413	4.575682	5.102585
32	O	3.372500	4.430839	4.902239	5.145773	6.012612
33	C	5.952225	5.206956	6.266676	4.355757	4.990845
34	H	6.348530	5.409951	6.433626	4.432170	4.939705
35	H	6.074310	5.095519	6.100964	4.117452	4.617959
36	H	6.748589	6.202071	7.272925	5.418785	6.069421
		16	17	18	19	20
16	C	0.000000				
17	H	1.084873	0.000000			
18	C	3.759146	4.123534	0.000000		
19	C	4.249107	4.900247	1.422657	0.000000	
20	C	5.628625	6.265432	2.453781	1.410447	0.000000
21	H	6.231837	6.983363	3.434670	2.161204	1.087793
22	C	6.417808	6.882131	2.822956	2.425857	1.385755
23	H	7.473349	7.954973	3.909578	3.411882	2.147579
24	C	6.106582	6.356833	2.434378	2.802324	2.420404
25	H	6.997429	7.140864	3.417227	3.888947	3.402013
26	C	4.903141	5.053170	1.416203	2.440110	2.804845
27	H	5.048049	4.962473	2.172963	3.428824	3.889947
28	C	4.336760	5.088263	4.322903	3.859175	4.834931
29	C	3.563439	3.853463	3.914253	4.242267	5.449470
30	O	3.782572	4.346986	4.615959	4.550794	5.724042
31	O	3.755304	3.723361	4.605228	5.193572	6.433411

32	O	5.125968	5.979007	5.262790	4.552480	5.359068
33	C	2.973231	2.629395	2.563112	3.842367	5.009074
34	H	3.092879	2.551848	3.045269	4.354507	5.458597
35	H	2.814245	2.296430	3.442508	4.571569	5.827646
36	H	4.041874	3.701871	2.736699	4.084330	5.053732

		21	22	23	24	25
21	H	0.000000				
22	C	2.151732	0.000000			
23	H	2.481647	1.086684	0.000000		
24	C	3.411020	1.409828	2.167478	0.000000	
25	H	4.306035	2.165884	2.492174	1.086773	0.000000
26	C	3.892603	2.427245	3.407922	1.385970	2.143691
27	H	4.977723	3.406150	4.296472	2.138199	2.456220
28	C	4.953658	5.966815	6.816737	6.280293	7.299968
29	C	5.983279	6.231545	7.225255	6.022045	6.906752
30	O	6.028573	6.739317	7.684063	6.790082	7.765121
31	O	7.059209	7.086814	8.105892	6.678925	7.471299
32	O	5.238043	6.599439	7.350647	7.109827	8.150923
33	C	5.961092	5.226746	6.287931	4.380795	5.018117
34	H	6.435533	5.566714	6.599264	4.620694	5.149242
35	H	6.709318	6.172452	7.242110	5.399440	6.054195
36	H	6.062174	5.040963	6.045105	4.037455	4.522592

		26	27	28	29	30
26	C	0.000000				
27	H	1.085236	0.000000			
28	C	5.573638	6.200782	0.000000		
29	C	4.963622	5.205078	2.279089	0.000000	
30	O	5.847349	6.259888	1.389273	1.408742	0.000000
31	O	5.501742	5.513741	3.413708	1.206263	2.276600
32	O	6.534217	7.247767	1.204035	3.420460	2.270425
33	C	2.997251	2.660385	4.977299	3.384122	4.505424
34	H	3.271048	2.761195	5.888043	4.388493	5.415332
35	H	4.028949	3.706861	4.841870	2.934210	4.084281
36	H	2.730531	2.181880	5.380755	3.720118	4.989126

		31	32	33	34	35
31	O	0.000000				
32	O	4.486206	0.000000			
33	C	3.349816	6.115467	0.000000		
34	H	4.286143	6.977005	1.099714	0.000000	
35	H	2.573660	5.986396	1.093228	1.774882	0.000000
36	H	3.655213	6.556786	1.092761	1.770599	1.761759

		36
36	H	0.000000

Stoichiometry C19H14O3
Framework group C1[X(C19H14O3)]
Deg. of freedom 102
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.596488	0.183481	-1.338712
2	6	0	-0.415553	1.149994	-0.993208
3	1	0	-0.337978	2.135618	-1.449015
4	6	0	0.526431	-1.080941	-0.687648
5	6	0	-0.574729	-1.310401	0.224014
6	6	0	0.061263	0.394138	1.750010
7	1	0	-0.739299	0.079708	2.404342
8	6	0	0.108094	1.584598	0.992854
9	1	0	-0.606815	2.393798	1.078775
10	6	0	1.683917	0.480442	-2.188863
11	1	0	1.740288	1.460079	-2.656210
12	6	0	2.660852	-0.470562	-2.426819
13	1	0	3.486107	-0.246195	-3.096951
14	6	0	2.595277	-1.726925	-1.789198
15	1	0	3.369445	-2.466510	-1.974868
16	6	0	1.559833	-2.022403	-0.919320
17	1	0	1.534154	-2.988812	-0.427035
18	6	0	-1.818348	-0.616516	-0.057605
19	6	0	-1.738240	0.648072	-0.704407
20	6	0	-2.910235	1.398074	-0.935244
21	1	0	-2.832292	2.370537	-1.416424
22	6	0	-4.148519	0.890475	-0.575642
23	1	0	-5.051345	1.459548	-0.780441
24	6	0	-4.237524	-0.368363	0.052865
25	1	0	-5.210581	-0.767755	0.326218
26	6	0	-3.093103	-1.101954	0.323158
27	1	0	-3.183706	-2.069235	0.806786
28	6	0	1.549792	1.935964	0.852323
29	6	0	1.442090	-0.016267	2.023409
30	8	0	2.302277	0.891700	1.375159
31	8	0	1.884214	-0.939364	2.661757
32	8	0	2.061662	2.913290	0.370117
33	6	0	-0.581853	-2.556366	1.072706
34	1	0	-0.813150	-3.443208	0.464937
35	1	0	0.391125	-2.713821	1.545642
36	1	0	-1.326777	-2.496005	1.869933

```
 Rotational constants (GHZ):      0.4485831      0.2705349
0.2636188
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   446 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   446 basis functions,   760 primitive gaussians,   446 cartesian
basis functions
    76 alpha electrons       76 beta electrons
       nuclear repulsion energy      1793.6322399165 Hartrees.
 NAtoms=   36 NActive=   36 NUniq=   36 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
```

```
 One-electron integrals computed using PRISM.
 NBasis=   446 RedAO= T  NBF=   446
 NBsUse=   441 1.00D-06 NBFU=   441
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -958.137842647     A.U. after   17 cycles
             Convg  =    0.4675D-08             -V/T =  2.0094
 Range of M.O.s used for correlation:     1   441
 NBasis=   446 NAE=    76 NBE=    76 NFC=     0 NFV=     0
 NROrb=    441 NOA=    76 NOB=    76 NVA=   365 NVB=   365

 **** Warning!!: The largest alpha MO coefficient is  0.14709298D+03

 Symmetrizing basis deriv contribution to polar:
 IMax=3 JMax=2 DiffMx= 0.00D+00
 G2DrvN: will do    37 centers at a time, making    1 passes doing
MaxLOS=2.
 Calling FoFCou, ICntrl=  3107 FMM=F I1Cent=   0 AccDes= 0.00D+00.
 FoFDir/FoFCou used for L=0 through L=2.
 End of G2Drv Frequency-dependent properties file   721 does not
exist.
 End of G2Drv Frequency-dependent properties file   722 does not
exist.
          IDoAtm=11111111111111111111111111111111111111
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
          There are   111 degrees of freedom in the 1st order CPHF.
IDoFFX=5.
    108 vectors produced by pass  0 Test12= 2.77D-14 1.00D-09 XBig12=
4.48D+02 9.51D+00.
 AX will form   108 AO Fock derivatives at one time.
    108 vectors produced by pass  1 Test12= 2.77D-14 1.00D-09 XBig12=
1.12D+02 1.61D+00.
    108 vectors produced by pass  2 Test12= 2.77D-14 1.00D-09 XBig12=
1.01D+00 1.08D-01.
    108 vectors produced by pass  3 Test12= 2.77D-14 1.00D-09 XBig12=
4.95D-03 7.89D-03.
    108 vectors produced by pass  4 Test12= 2.77D-14 1.00D-09 XBig12=
1.27D-05 3.27D-04.
    105 vectors produced by pass  5 Test12= 2.77D-14 1.00D-09 XBig12=
1.59D-08 9.16D-06.
     37 vectors produced by pass  6 Test12= 2.77D-14 1.00D-09 XBig12=
6.82D-11 8.96D-07.
     36 vectors produced by pass  7 Test12= 2.77D-14 1.00D-09 XBig12=
9.33D-12 2.49D-07.
```

This journal is © The Royal Society of Chemistry 2014

```
     35 vectors produced by pass  8 Test12= 2.77D-14 1.00D-09 XBig12=
7.83D-13 5.41D-08.
     25 vectors produced by pass  9 Test12= 2.77D-14 1.00D-09 XBig12=
1.40D-14 9.62D-09.
     14 vectors produced by pass 10 Test12= 2.77D-14 1.00D-09 XBig12=
4.24D-16 1.85D-09.
      5 vectors produced by pass 11 Test12= 2.77D-14 1.00D-09 XBig12=
4.46D-16 1.45D-09.
      2 vectors produced by pass 12 Test12= 2.77D-14 1.00D-09 XBig12=
3.14D-16 1.54D-09.
      2 vectors produced by pass 13 Test12= 2.77D-14 1.00D-09 XBig12=
2.51D-16 1.13D-09.
      2 vectors produced by pass 14 Test12= 2.77D-14 1.00D-09 XBig12=
6.94D-16 2.29D-09.
      1 vectors produced by pass 15 Test12= 2.77D-14 1.00D-09 XBig12=
3.37D-16 1.18D-09.
 Inverted reduced A of dimension   804 with in-core refinement.
 Isotropic polarizability for W=    0.000000      239.07 Bohr**3.
 End of Minotr Frequency-dependent properties file   721 does not
exist.
 End of Minotr Frequency-dependent properties file   722 does not
exist.


**********************************************************************

            Population analysis using the SCF density.

**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.21462 -19.16292 -19.16005 -10.33593 -
10.33229
 Alpha  occ. eigenvalues --  -10.25475 -10.24026 -10.23750 -10.22720 -
10.22718
 Alpha  occ. eigenvalues --  -10.22648 -10.22303 -10.22240 -10.21890 -
10.21873
 Alpha  occ. eigenvalues --  -10.21829 -10.21765 -10.21142 -10.21108 -
10.21052
 Alpha  occ. eigenvalues --  -10.21011 -10.20464  -1.13339  -1.06938
-1.03089
 Alpha  occ. eigenvalues --   -0.91435  -0.87496  -0.83759  -0.82590
-0.81170
 Alpha  occ. eigenvalues --   -0.77328  -0.76472  -0.74699  -0.71006
-0.69044
 Alpha  occ. eigenvalues --   -0.66958  -0.63534  -0.62540  -0.61760
-0.60313
 Alpha  occ. eigenvalues --   -0.57890  -0.56315  -0.54530  -0.52511
-0.50361
 Alpha  occ. eigenvalues --   -0.49530  -0.48791  -0.48417  -0.47338
-0.46892
 Alpha  occ. eigenvalues --   -0.46116  -0.45472  -0.45281  -0.44461
-0.43707
 Alpha  occ. eigenvalues --   -0.43470  -0.43119  -0.41937  -0.41208
-0.40452
 Alpha  occ. eigenvalues --   -0.39934  -0.39785  -0.39643  -0.38119
-0.37123
 Alpha  occ. eigenvalues --   -0.35636  -0.35100  -0.34749  -0.32670
-0.31188
 Alpha  occ. eigenvalues --   -0.30890  -0.28467  -0.27491  -0.26670
-0.26394
 Alpha  occ. eigenvalues --   -0.23358
 Alpha virt. eigenvalues --   -0.09485  -0.07464  -0.03330  -0.02628
-0.00952
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --   -0.00775   0.00151   0.00259   0.00476
0.01351
 Alpha virt. eigenvalues --    0.02113   0.02219   0.03246   0.03648
0.03763
 Alpha virt. eigenvalues --    0.04192   0.04495   0.04686   0.06125
0.06340
 Alpha virt. eigenvalues --    0.06545   0.06563   0.06935   0.07328
0.07715
 Alpha virt. eigenvalues --    0.08487   0.09122   0.09551   0.09858
0.10342
 Alpha virt. eigenvalues --    0.10667   0.11298   0.11339   0.11635
0.12096
 Alpha virt. eigenvalues --    0.12253   0.12879   0.13366   0.13786
0.14091
 Alpha virt. eigenvalues --    0.14217   0.14655   0.14901   0.15697
0.15727
 Alpha virt. eigenvalues --    0.15975   0.16159   0.16190   0.16847
0.16963
 Alpha virt. eigenvalues --    0.17573   0.17672   0.17950   0.18523
0.18600
 Alpha virt. eigenvalues --    0.18878   0.19465   0.19666   0.20011
0.20099
 Alpha virt. eigenvalues --    0.20250   0.20515   0.21018   0.21307
0.21590
 Alpha virt. eigenvalues --    0.22085   0.22394   0.22730   0.22928
0.23459
 Alpha virt. eigenvalues --    0.23488   0.23818   0.24247   0.24924
0.25218
 Alpha virt. eigenvalues --    0.25302   0.25407   0.25733   0.26214
0.26792
 Alpha virt. eigenvalues --    0.26878   0.27057   0.27273   0.27977
0.28275
 Alpha virt. eigenvalues --    0.28464   0.28844   0.29172   0.29341
0.29530
 Alpha virt. eigenvalues --    0.29655   0.29793   0.30217   0.30859
0.31129
 Alpha virt. eigenvalues --    0.32104   0.32721   0.33260   0.33497
0.34185
 Alpha virt. eigenvalues --    0.34707   0.35265   0.35515   0.36009
0.36133
 Alpha virt. eigenvalues --    0.36405   0.37146   0.37471   0.37766
0.38579
 Alpha virt. eigenvalues --    0.39416   0.39910   0.40117   0.41245
0.41550
 Alpha virt. eigenvalues --    0.43020   0.43352   0.43632   0.44375
0.45643
 Alpha virt. eigenvalues --    0.46263   0.46947   0.47626   0.48695
0.52008
 Alpha virt. eigenvalues --    0.52770   0.56483   0.57573   0.58090
0.59948
 Alpha virt. eigenvalues --    0.62157   0.64906   0.65765   0.67158
0.69035
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.69442   0.69995   0.70215   0.71576
0.71688
 Alpha virt. eigenvalues --    0.72643   0.72959   0.73372   0.74242
0.75215
 Alpha virt. eigenvalues --    0.75439   0.75994   0.76318   0.76708
0.77698
 Alpha virt. eigenvalues --    0.78292   0.78453   0.80054   0.80485
0.81077
 Alpha virt. eigenvalues --    0.81910   0.82193   0.83249   0.83306
0.83996
 Alpha virt. eigenvalues --    0.85343   0.87392   0.88323   0.89504
0.89905
 Alpha virt. eigenvalues --    0.90628   0.91233   0.92003   0.92914
0.93502
 Alpha virt. eigenvalues --    0.94011   0.94077   0.94508   0.95997
0.96238
 Alpha virt. eigenvalues --    0.96977   0.97878   0.99664   1.00475
1.01155
 Alpha virt. eigenvalues --    1.02313   1.02862   1.03364   1.04887
1.06778
 Alpha virt. eigenvalues --    1.08099   1.08508   1.09427   1.10296
1.11325
 Alpha virt. eigenvalues --    1.12557   1.13733   1.14320   1.15145
1.17240
 Alpha virt. eigenvalues --    1.17315   1.18461   1.19813   1.19987
1.21354
 Alpha virt. eigenvalues --    1.21751   1.22417   1.24345   1.25316
1.25633
 Alpha virt. eigenvalues --    1.27009   1.28696   1.29298   1.29608
1.30306
 Alpha virt. eigenvalues --    1.31692   1.33477   1.34127   1.35064
1.36674
 Alpha virt. eigenvalues --    1.37241   1.38165   1.39915   1.40377
1.41903
 Alpha virt. eigenvalues --    1.42065   1.42689   1.43768   1.44265
1.44900
 Alpha virt. eigenvalues --    1.45480   1.46698   1.46848   1.47371
1.47777
 Alpha virt. eigenvalues --    1.48270   1.50204   1.50589   1.52059
1.52857
 Alpha virt. eigenvalues --    1.53760   1.54454   1.56194   1.57712
1.62212
 Alpha virt. eigenvalues --    1.66664   1.67388   1.69425   1.71546
1.73368
 Alpha virt. eigenvalues --    1.74762   1.77706   1.79175   1.80951
1.81268
 Alpha virt. eigenvalues --    1.82162   1.83404   1.84101   1.84575
1.85691
 Alpha virt. eigenvalues --    1.86571   1.87857   1.88308   1.89312
1.89837
 Alpha virt. eigenvalues --    1.90525   1.93041   1.94199   1.94824
1.96138
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    1.96749   1.97375   1.98475   1.99069
2.00214
 Alpha virt. eigenvalues --    2.01682   2.03296   2.04962   2.06717
2.07669
 Alpha virt. eigenvalues --    2.08553   2.09569   2.10630   2.10968
2.12250
 Alpha virt. eigenvalues --    2.15122   2.15914   2.17554   2.19115
2.19469
 Alpha virt. eigenvalues --    2.20021   2.21652   2.22788   2.24975
2.26072
 Alpha virt. eigenvalues --    2.26736   2.27444   2.29048   2.30258
2.31036
 Alpha virt. eigenvalues --    2.32033   2.33283   2.33643   2.34264
2.36403
 Alpha virt. eigenvalues --    2.37500   2.40625   2.41003   2.42644
2.47543
 Alpha virt. eigenvalues --    2.49182   2.50468   2.50718   2.56304
2.58193
 Alpha virt. eigenvalues --    2.61282   2.61906   2.62627   2.64500
2.66165
 Alpha virt. eigenvalues --    2.66646   2.68855   2.70216   2.72047
2.74114
 Alpha virt. eigenvalues --    2.75082   2.75978   2.79846   2.80968
2.83153
 Alpha virt. eigenvalues --    2.85106   2.86492   2.86910   2.89116
2.90322
 Alpha virt. eigenvalues --    2.91009   2.94880   2.95792   2.98843
3.11059
 Alpha virt. eigenvalues --    3.12257   3.16988   3.23078   3.24812
3.25129
 Alpha virt. eigenvalues --    3.33607   3.40977   3.42925   4.24793
4.29549
 Alpha virt. eigenvalues --    4.30928   4.32053   4.34815   4.36751
4.37426
 Alpha virt. eigenvalues --    4.39648   4.41691   4.47141   4.48014
4.50259
 Alpha virt. eigenvalues --    4.51984   4.52864   4.55389   4.62629
4.68069
 Alpha virt. eigenvalues --    4.69557   4.75625   4.84794   4.93027
5.28673
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   26.144200 -19.299097  -0.003227  12.246382  -9.744127  -
0.515075
     2  C  -19.299097  41.881439   0.214613 -17.194853  16.309132
0.287496
     3  H   -0.003227   0.214613   0.527568   0.037266  -0.016044
0.014151
     4  C   12.246382 -17.194853   0.037266  43.215808 -13.426185  -
0.416732
     5  C   -9.744127  16.309132  -0.016044 -13.426185  29.544227
0.407083
```

This journal is © The Royal Society of Chemistry 2014

```
     6  C   -0.515075   0.287496   0.014151  -0.416732   0.407083
9.385267
     7  H    0.019500  -0.011972  -0.000049  -0.012373  -0.009282
0.329465
     8  C    1.455390  -2.266281   0.002658   0.789079  -1.660710  -
2.124148
     9  H    0.026106  -0.075792  -0.001948   0.020963  -0.015627  -
0.023219
    10  C   -6.395797   5.280316   0.021894  -6.282881   1.407946
0.461682
    11  H   -0.064310  -0.019961   0.003974   0.071141   0.017867
0.005605
    12  C   -2.926605   0.570927   0.004838  -1.402157   0.780327
0.005950
    13  H    0.011479  -0.014568  -0.000007   0.021788   0.006424
0.001288
    14  C    0.955749  -0.521870   0.005842   0.460848  -0.943347
0.193637
    15  H    0.022638   0.002292   0.000000   0.013948  -0.014920  -
0.002369
    16  C   -5.307836   6.057683  -0.003563 -19.782932   5.073217
0.984267
    17  H    0.036093   0.005095   0.000002  -0.150191   0.013539  -
0.009263
    18  C    5.690916 -14.851597   0.012555   4.991994 -12.366154  -
1.353371
    19  C    8.343135 -17.810436  -0.007232   7.286716 -10.748224  -
0.902416
    20  C   -0.154250   1.447208  -0.007956  -1.007141  -1.082871  -
0.188048
    21  H   -0.016657  -0.007954   0.003742  -0.002005   0.007291  -
0.000795
    22  C   -0.559623   0.114865  -0.008970  -0.033739   0.510296  -
0.103954
    23  H   -0.002622  -0.002174  -0.000007   0.000234   0.001654
0.000128
    24  C    0.190708  -0.281830   0.001100  -0.229323  -1.097255
0.044926
    25  H    0.000843   0.001697   0.000000  -0.002038  -0.004895
0.000021
    26  C   -1.708819   2.555439   0.007330  -0.668912   2.530830  -
0.037902
    27  H    0.001709   0.000512   0.000002   0.026356   0.062335
0.002742
    28  C   -1.049842   1.930915  -0.028525  -0.697241   0.940227
0.996099
    29  C   -0.228630   0.414936  -0.000341  -0.247353   0.676886  -
1.833860
    30  O   -0.127581   0.121573   0.000075  -0.004527   0.043074  -
0.233389
    31  O    0.050889  -0.060356   0.000030   0.328486  -0.138309  -
0.107796
```

This journal is © The Royal Society of Chemistry 2014

32	O	0.163403	-0.152795	0.005119	0.040428	-0.045720	-0.064175
33	C	-0.877120	1.039028	0.003327	-2.215070	-0.191268	0.667491
34	H	-0.014722	0.033586	0.000000	-0.175037	-0.006353	0.018261
35	H	-0.014389	-0.024220	0.000000	-0.209052	0.006564	-0.007176
36	H	0.005975	-0.015022	0.000000	0.207366	-0.054832	-0.012534

		7	8	9	10	11	12
1	C	0.019500	1.455390	0.026106	-6.395797	-0.064310	-2.926605
2	C	-0.011972	-2.266281	-0.075792	5.280316	-0.019961	0.570927
3	H	-0.000049	0.002658	-0.001948	0.021894	0.003974	0.004838
4	C	-0.012373	0.789079	0.020963	-6.282881	0.071141	-1.402157
5	C	-0.009282	-1.660710	-0.015627	1.407946	0.017867	0.780327
6	C	0.329465	-2.124148	-0.023219	0.461682	0.005605	0.005950
7	H	0.474435	0.000174	-0.002134	-0.005264	0.000000	0.000452
8	C	0.000174	9.400553	0.381801	-0.057940	-0.012232	0.106880
9	H	-0.002134	0.381801	0.477026	0.005326	-0.000001	-0.001164
10	C	-0.005264	-0.057940	0.005326	11.528949	0.261198	1.058378
11	H	0.000000	-0.012232	-0.000001	0.261198	0.531244	0.084017
12	C	0.000452	0.106880	-0.001164	1.058378	0.084017	7.873930
13	H	0.000000	-0.002560	0.000000	-0.006729	-0.004315	0.292858
14	C	-0.000163	-0.139273	0.001024	-0.862532	0.002621	0.462473
15	H	0.000000	0.001854	0.000000	0.021669	-0.000164	-0.051415
16	C	0.008148	-0.212971	-0.000465	5.130845	-0.021515	1.035439
17	H	0.000001	0.004402	0.000000	-0.019304	0.000016	0.013945
18	C	0.072201	1.603138	0.020251	-1.906507	-0.006194	-0.305434
19	C	0.016895	0.893252	0.059142	-2.622268	-0.051335	-1.032488
20	C	0.000973	-0.088212	-0.034349	-0.875911	0.002425	-0.133153

This journal is © The Royal Society of Chemistry 2014

21	H	0.000000	0.002736	-0.000023	0.004990	0.000002
0.000693						
22	C	-0.004447	-0.009157	-0.018703	-0.152087	-0.000220
0.025853						
23	H	0.000000	-0.000426	0.000002	0.000221	0.000000
0.000003						
24	C	-0.003937	-0.013944	0.007379	0.064726	-0.000114
0.011200						
25	H	0.000000	-0.000151	0.000000	-0.000102	0.000000
0.000005						
26	C	-0.043129	-0.481891	-0.006140	-0.466914	0.000214
0.127154						
27	H	-0.000073	-0.002294	0.000000	0.000775	0.000000
0.000024						
28	C	0.010447	-1.774952	-0.086955	0.089153	0.010317
0.079814						
29	C	-0.067232	0.916599	0.014620	-0.155292	-0.003289
0.001091						
30	O	0.008608	-0.387648	0.007958	-0.012920	0.000351
0.022811						
31	O	0.001916	-0.047373	-0.000691	0.002292	-0.000002
0.008622						
32	O	-0.000571	-0.056042	0.001313	-0.079464	0.000073
0.043536						
33	C	-0.023785	-0.094119	-0.003356	0.479170	0.000309
0.147517						
34	H	-0.000034	-0.009447	0.000001	0.005517	0.000000
0.001469						
35	H	0.000081	0.016806	-0.000003	-0.003135	0.000000
0.005098						
36	H	0.001272	0.003087	-0.000005	-0.000253	0.000000
0.000205						

		13	14	15	16	17	18
1	C	0.011479	0.955749	0.022638	-5.307836	0.036093	
5.690916							
2	C	-0.014568	-0.521870	0.002292	6.057683	0.005095	
14.851597							
3	H	-0.000007	0.005842	0.000000	-0.003563	0.000002	
0.012555							
4	C	0.021788	0.460848	0.013948	-19.782932	-0.150191	
4.991994							
5	C	0.006424	-0.943347	-0.014920	5.073217	0.013539	
12.366154							
6	C	0.001288	0.193637	-0.002369	0.984267	-0.009263	
1.353371							
7	H	0.000000	-0.000163	0.000000	0.008148	0.000001	
0.072201							
8	C	-0.002560	-0.139273	0.001854	-0.212971	0.004402	
1.603138							
9	H	0.000000	0.001024	0.000000	-0.000465	0.000000	
0.020251							

This journal is © The Royal Society of Chemistry 2014

```
    10  C   -0.006729  -0.862532   0.021669   5.130845  -0.019304  -
1.906507
    11  H   -0.004315   0.002621  -0.000164  -0.021515   0.000016  -
0.006194
    12  C    0.292858   0.462473  -0.051415   1.035439   0.013945  -
0.305434
    13  H    0.523846  -0.034286  -0.004164   0.019161  -0.000166
0.001505
    14  C   -0.034286   7.475690   0.256328  -1.024139   0.087161  -
0.135516
    15  H   -0.004164   0.256328   0.525521   0.047011  -0.004672  -
0.001636
    16  C    0.019161  -1.024139   0.047011  22.162044   0.300231  -
2.740073
    17  H   -0.000166   0.087161  -0.004672   0.300231   0.537206  -
0.001322
    18  C    0.001505  -0.135516  -0.001636  -2.740073  -0.001322
36.964126
    19  C   -0.002983  -0.011726   0.003386  -4.630028   0.001375
10.424931
    20  C    0.000104  -0.020219  -0.000074  -0.662340   0.000650  -
3.665818
    21  H    0.000000  -0.000136   0.000000   0.000113   0.000000
0.058610
    22  C   -0.000011  -0.001938   0.000019  -0.203465   0.000041  -
1.079215
    23  H    0.000000   0.000004   0.000000  -0.000147   0.000000
0.003405
    24  C    0.000020  -0.024180  -0.000001   0.187418  -0.001086
2.642621
    25  H    0.000000   0.000007   0.000000   0.000206   0.000000
0.008820
    26  C   -0.000202  -0.055018   0.000068  -1.498327  -0.004639 -
14.437947
    27  H    0.000000  -0.000313   0.000000  -0.003593   0.000001  -
0.173047
    28  C    0.003972   0.094276  -0.002136   0.211295  -0.002640  -
0.804727
    29  C   -0.001663  -0.128694   0.003272  -0.389852   0.009263
0.159735
    30  O   -0.000057   0.016899  -0.000007  -0.014569   0.000114  -
0.043673
    31  O    0.000003  -0.020134  -0.000088  -0.147877  -0.000654  -
0.068831
    32  O   -0.000095   0.000469  -0.000001  -0.025028  -0.000001
0.028722
    33  C    0.000281   0.202355  -0.003492   1.862016  -0.005669  -
2.943061
    34  H    0.000000   0.011138  -0.000002   0.095925  -0.001020  -
0.158962
    35  H    0.000000  -0.012187  -0.000002   0.032405  -0.000812
0.204591
```

This journal is © The Royal Society of Chemistry 2014

36	H	0.000000	0.003489	0.000000	-0.024387	0.000160	-0.232211

		19	20	21	22	23	24
1	C	8.343135	-0.154250	-0.016657	-0.559623	-0.002622	0.190708
2	C	-17.810436	1.447208	-0.007954	0.114865	-0.002174	-0.281830
3	H	-0.007232	-0.007956	0.003742	-0.008970	-0.000007	0.001100
4	C	7.286716	-1.007141	-0.002005	-0.033739	0.000234	-0.229323
5	C	-10.748224	-1.082871	0.007291	0.510296	0.001654	-1.097255
6	C	-0.902416	-0.188048	-0.000795	-0.103954	0.000128	0.044926
7	H	0.016895	0.000973	0.000000	-0.004447	0.000000	-0.003937
8	C	0.893252	-0.088212	0.002736	-0.009157	-0.000426	-0.013944
9	H	0.059142	-0.034349	-0.000023	-0.018703	0.000002	0.007379
10	C	-2.622268	-0.875911	0.004990	-0.152087	0.000221	0.064726
11	H	-0.051335	0.002425	0.000002	-0.000220	0.000000	-0.000114
12	C	-1.032488	-0.133153	0.000693	-0.025853	0.000003	0.011200
13	H	-0.002983	0.000104	0.000000	-0.000011	0.000000	0.000020
14	C	-0.011726	-0.020219	-0.000136	-0.001938	0.000004	-0.024180
15	H	0.003386	-0.000074	0.000000	0.000019	0.000000	-0.000001
16	C	-4.630028	-0.662340	0.000113	-0.203465	-0.000147	0.187418
17	H	0.001375	0.000650	0.000000	0.000041	0.000000	-0.001086
18	C	10.424931	-3.665818	0.058610	-1.079215	0.003405	2.642621
19	C	23.780839	-1.710714	-0.042487	-1.704564	0.012765	0.744773
20	C	-1.710714	10.680824	0.263354	0.395512	0.006752	-0.851034
21	H	-0.042487	0.263354	0.534961	0.031651	-0.004309	0.006359
22	C	-1.704564	0.395512	0.031651	7.612669	0.300028	0.152088
23	H	0.012765	0.006752	-0.004309	0.300028	0.523974	-0.037714
24	C	0.744773	-0.851034	0.006359	0.152088	-0.037714	7.456851

This journal is © The Royal Society of Chemistry 2014

25	H	0.003113	0.011858	-0.000160	-0.037794	-0.004074
0.284241						
26	C	-1.354223	3.393729	-0.027938	0.999486	0.013699
2.993312						
27	H	0.011210	-0.025126	0.000017	0.019732	-0.000165
0.045328						
28	C	-0.783336	-0.009788	0.003758	0.124045	0.000091
0.040795						
29	C	0.116318	0.088951	-0.001050	0.004099	-0.000047
0.055672						
30	O	-0.042720	0.024164	0.000004	0.002126	0.000000
0.001520						
31	O	0.027796	0.000595	0.000000	0.000895	0.000000
0.004972						
32	O	0.074018	0.016146	0.000001	-0.001277	0.000000
0.000264						
33	C	-1.920556	-0.046379	0.000160	-0.123531	0.000486
0.063371						
34	H	-0.035104	0.000491	0.000000	-0.000959	0.000000
0.009317						
35	H	0.013247	0.000332	0.000000	-0.000593	0.000000
0.004123						
36	H	-0.026526	-0.006502	0.000000	0.004105	0.000000
0.011271						

		25	26	27	28	29	30
1	C	0.000843	-1.708819	0.001709	-1.049842	-0.228630	
0.127581							
2	C	0.001697	2.555439	0.000512	1.930915	0.414936	
0.121573							
3	H	0.000000	0.007330	0.000002	-0.028525	-0.000341	
0.000075							
4	C	-0.002038	-0.668912	0.026356	-0.697241	-0.247353	
0.004527							
5	C	-0.004895	2.530830	0.062335	0.940227	0.676886	
0.043074							
6	C	0.000021	-0.037902	0.002742	0.996099	-1.833860	
0.233389							
7	H	0.000000	-0.043129	-0.000073	0.010447	-0.067232	
0.008608							
8	C	-0.000151	-0.481891	-0.002294	-1.774952	0.916599	
0.387648							
9	H	0.000000	-0.006140	0.000000	-0.086955	0.014620	
0.007958							
10	C	-0.000102	-0.466914	0.000775	0.089153	-0.155292	
0.012920							
11	H	0.000000	0.000214	0.000000	0.010317	-0.003289	
0.000351							
12	C	0.000005	-0.127154	-0.000024	-0.079814	-0.001091	
0.022811							
13	H	0.000000	-0.000202	0.000000	0.003972	-0.001663	
0.000057							

```
    14  C    0.000007  -0.055018  -0.000313   0.094276  -0.128694
0.016899
    15  H    0.000000   0.000068   0.000000  -0.002136   0.003272  -
0.000007
    16  C    0.000206  -1.498327  -0.003593   0.211295  -0.389852  -
0.014569
    17  H    0.000000  -0.004639   0.000001  -0.002640   0.009263
0.000114
    18  C    0.008820 -14.437947  -0.173047  -0.804727   0.159735  -
0.043673
    19  C    0.003113  -1.354223   0.011210  -0.783336   0.116318  -
0.042720
    20  C    0.011858   3.393729  -0.025126  -0.009788   0.088951
0.024164
    21  H   -0.000160  -0.027938   0.000017   0.003758  -0.001050
0.000004
    22  C   -0.037794   0.999486   0.019732   0.124045   0.004099
0.002126
    23  H   -0.004074   0.013699  -0.000165   0.000091  -0.000047
0.000000
    24  C    0.284241  -2.993312   0.045328  -0.040795   0.055672  -
0.001520
    25  H    0.525628   0.032161  -0.004594  -0.000072   0.000111
0.000000
    26  C    0.032161  19.765236   0.324301   0.027131   0.271533
0.027144
    27  H   -0.004594   0.324301   0.538114  -0.000494   0.001277
0.000001
    28  C   -0.000072   0.027131  -0.000494   6.898801  -1.056629
0.346572
    29  C    0.000111   0.271533   0.001277  -1.056629   6.944741
0.263353
    30  O    0.000000   0.027144   0.000001   0.346572   0.263353
8.315505
    31  O    0.000000   0.008160   0.000007   0.018424   0.453839  -
0.068440
    32  O    0.000000   0.001669   0.000000   0.420817   0.041839  -
0.088225
    33  C   -0.001401   0.143670  -0.011164   0.070514  -0.391928
0.017573
    34  H    0.000000   0.048085  -0.000569   0.001482   0.000320
0.000020
    35  H    0.000000  -0.025431   0.000096  -0.003534  -0.004866  -
0.000363
    36  H    0.000002   0.033668   0.001051  -0.000822  -0.003404  -
0.000055
              31         32         33         34         35         36
     1  C    0.050889   0.163403  -0.877120  -0.014722  -0.014389
0.005975
     2  C   -0.060356  -0.152795   1.039028   0.033586  -0.024220  -
0.015022
```

This journal is © The Royal Society of Chemistry 2014

```
     3  H    0.000030   0.005119   0.003327   0.000000   0.000000
0.000000
     4  C    0.328486   0.040428  -2.215070  -0.175037  -0.209052
0.207366
     5  C   -0.138309  -0.045720  -0.191268  -0.006353   0.006564  -
0.054832
     6  C   -0.107796  -0.064175   0.667491   0.018261  -0.007176  -
0.012534
     7  H    0.001916  -0.000571  -0.023785  -0.000034   0.000081
0.001272
     8  C   -0.047373  -0.056042  -0.094119  -0.009447   0.016806
0.003087
     9  H   -0.000691   0.001313  -0.003356   0.000001  -0.000003  -
0.000005
    10  C    0.002292  -0.079464   0.479170   0.005517  -0.003135  -
0.000253
    11  H   -0.000002   0.000073   0.000309   0.000000   0.000000
0.000000
    12  C   -0.008622  -0.043536   0.147517  -0.001469   0.005098  -
0.000205
    13  H    0.000003  -0.000095   0.000281   0.000000   0.000000
0.000000
    14  C   -0.020134   0.000469   0.202355   0.011138  -0.012187
0.003489
    15  H   -0.000088  -0.000001  -0.003492  -0.000002  -0.000002
0.000000
    16  C   -0.147877  -0.025028   1.862016   0.095925   0.032405  -
0.024387
    17  H   -0.000654  -0.000001  -0.005669  -0.001020  -0.000812
0.000160
    18  C   -0.068831   0.028722  -2.943061  -0.158962   0.204591  -
0.232211
    19  C    0.027796   0.074018  -1.920556  -0.035104   0.013247  -
0.026526
    20  C    0.000595   0.016146  -0.046379   0.000491   0.000332  -
0.006502
    21  H    0.000000   0.000001   0.000160   0.000000   0.000000
0.000000
    22  C    0.000895  -0.001277  -0.123531  -0.000959  -0.000593
0.004105
    23  H    0.000000   0.000000   0.000486   0.000000   0.000000
0.000000
    24  C   -0.004972   0.000264  -0.063371   0.009317   0.004123  -
0.011271
    25  H    0.000000   0.000000  -0.001401   0.000000   0.000000
0.000002
    26  C    0.008160   0.001669   0.143670   0.048085  -0.025431
0.033668
    27  H    0.000007   0.000000  -0.011164  -0.000569   0.000096
0.001051
    28  C    0.018424   0.420817   0.070514   0.001482  -0.003534  -
0.000822
```

This journal is © The Royal Society of Chemistry 2014

```
    29  C    0.453839   0.041839  -0.391928   0.000320  -0.004866  -
0.003404
    30  O   -0.068440  -0.088225   0.017573   0.000020  -0.000363  -
0.000055
    31  O    8.169428   0.000014  -0.001442  -0.000160  -0.003707
0.002019
    32  O    0.000014   8.152233   0.000535  -0.000001   0.000017  -
0.000001
    33  C   -0.001442   0.000535   9.365804   0.499602   0.354975
0.449312
    34  H   -0.000160  -0.000001   0.499602   0.489570  -0.027244  -
0.026783
    35  H   -0.003707   0.000017   0.354975  -0.027244   0.433347  -
0.020344
    36  H    0.002019  -0.000001   0.449312  -0.026783  -0.020344
0.498228
 Mulliken atomic charges:
              1
     1  C   -0.354786
     2  C    0.342025
     3  H    0.211779
     4  C    0.400938
     5  C   -0.772796
     6  C    0.130661
     7  H    0.239877
     8  C   -0.136638
     9  H    0.247666
    10  C    0.080253
    11  H    0.192277
    12  C   -0.337559
    13  H    0.189079
    14  C   -0.294338
    15  H    0.187139
    16  C   -0.514316
    17  H    0.192145
    18  C    0.387173
    19  C   -0.373546
    20  C    0.235820
    21  H    0.185070
    22  C   -0.201559
    23  H    0.188240
    24  C   -0.253455
    25  H    0.186567
    26  C   -0.245656
    27  H    0.185888
    28  C    0.223967
    29  C    0.077857
    30  O   -0.192230
    31  O   -0.385337
    32  O   -0.390146
    33  C   -0.387413
    34  H    0.244552
```

This journal is © The Royal Society of Chemistry 2014

```
    35  H    0.285377
    36  H    0.225424
 Sum of Mulliken atomic charges =   0.00000
 Mulliken charges with hydrogens summed into heavy atoms:
               1
     1  C   -0.354786
     2  C    0.553804
     4  C    0.400938
     5  C   -0.772796
     6  C    0.370539
     8  C    0.111028
    10  C    0.272530
    12  C   -0.148480
    14  C   -0.107199
    16  C   -0.322171
    18  C    0.387173
    19  C   -0.373546
    20  C    0.420890
    22  C   -0.013318
    24  C   -0.066888
    26  C   -0.059768
    28  C    0.223967
    29  C    0.077857
    30  O   -0.192230
    31  O   -0.385337
    32  O   -0.390146
    33  C    0.367939
 Sum of Mulliken charges with hydrogens summed into heavy atoms =
0.00000
 APT atomic charges:
               1
     1  C   -0.057950
     2  C    0.165780
     3  H    0.010999
     4  C   -0.124245
     5  C    0.427828
     6  C   -0.337334
     7  H    0.046118
     8  C   -0.134941
     9  H    0.024665
    10  C   -0.007594
    11  H    0.037320
    12  C   -0.020679
    13  H    0.030162
    14  C   -0.015836
    15  H    0.027138
    16  C   -0.012740
    17  H    0.039115
    18  C   -0.099890
    19  C   -0.036898
    20  C   -0.018675
    21  H    0.030519
```

This journal is © The Royal Society of Chemistry 2014

```
    22  C   -0.032459
    23  H    0.027504
    24  C   -0.033387
    25  H    0.024601
    26  C   -0.017561
    27  H    0.037162
    28  C    1.071769
    29  C    1.131710
    30  O   -0.740541
    31  O   -0.733241
    32  O   -0.721539
    33  C   -0.033441
    34  H   -0.005998
    35  H    0.042008
    36  H    0.010553
Sum of APT charges=   0.00000
APT Atomic charges with hydrogens summed into heavy atoms:
              1
     1  C   -0.057950
     2  C    0.176779
     3  H    0.000000
     4  C   -0.124245
     5  C    0.427828
     6  C   -0.291216
     7  H    0.000000
     8  C   -0.110277
     9  H    0.000000
    10  C    0.029726
    11  H    0.000000
    12  C    0.009483
    13  H    0.000000
    14  C    0.011302
    15  H    0.000000
    16  C    0.026375
    17  H    0.000000
    18  C   -0.099890
    19  C   -0.036898
    20  C    0.011844
    21  H    0.000000
    22  C   -0.004954
    23  H    0.000000
    24  C   -0.008786
    25  H    0.000000
    26  C    0.019601
    27  H    0.000000
    28  C    1.071769
    29  C    1.131710
    30  O   -0.740541
    31  O   -0.733241
    32  O   -0.721539
    33  C    0.013123
    34  H    0.000000
```

```
    35  H    0.000000
    36  H    0.000000
 Sum of APT charges=   0.00000
 Electronic spatial extent (au):  <R**2>=           5041.1419
 Charge=              0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=             -5.4086    Y=             -1.5840    Z=
-2.2503  Tot=              6.0684
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=           -126.8744   YY=           -126.2592   ZZ=           -
131.6991
   XY=             -8.1627   XZ=            -13.3802   YZ=
-1.2778
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=              1.4032   YY=              2.0183   ZZ=
-3.4215
   XY=             -8.1627   XZ=            -13.3802   YZ=
-1.2778
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=            -45.2058  YYY=            -32.5972  ZZZ=
1.4672  XYY=            -23.6543
  XXY=            -17.2908  XXZ=            -29.5914  XZZ=
6.1500  YZZ=             26.4858
  YYZ=             -0.8551  XYZ=             18.7637
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=          -3413.8637 YYYY=          -1733.8866 ZZZZ=          -
1633.6594 XXXY=            -66.8150
 XXXZ=            -90.2713 YYYX=            -89.9419 YYYZ=
-28.9219 ZZZX=            -65.2384
 ZZZY=              7.1675 XXYY=           -900.1249 XXZZ=           -
885.0444 YYZZ=           -538.5710
 XXYZ=            -14.7063 YYXZ=            -12.2265 ZZXY=
35.1891
 N-N= 1.793632239917D+03 E-N=-5.812676729375D+03  KE=
9.491772442919D+02
  Exact polarizability: 296.412  -8.627 224.088 -13.899 -14.103
196.706
 Approx polarizability: 471.760 -10.856 424.792 -18.469 -46.235
349.919
 Calling FoFJK, ICntrl=    100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 Full mass-weighted force constant matrix:
 Low frequencies --- -439.8290  -12.8700   -4.5761   -0.0001    0.0014
0.0014
 Low frequencies ---    9.7126   53.3786   75.8431
 ******    1 imaginary frequencies (negative Signs) ******
 Diagonal vibrational polarizability:
       18.4742028      31.2725833      39.1552086
 Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman
scattering
 activities (A**4/AMU), depolarization ratios for plane and
unpolarized
```

This journal is © The Royal Society of Chemistry 2014

incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-439.8283	53.3320	75.8368
Red. masses --	9.8088	9.5129	6.8216
Frc consts --	1.1180	0.0159	0.0231
IR Inten --	1.8578	1.9899	3.2896

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.04	-0.01	0.03	-0.02	0.05	-0.05	-0.03	0.02	0.03
2	6	0.15	0.14	0.48	-0.03	0.03	-0.01	-0.05	0.01	0.02
3	1	0.08	0.06	0.28	-0.07	0.02	-0.03	-0.05	0.01	0.02
4	6	0.04	0.02	-0.01	0.03	0.05	-0.04	-0.02	0.02	0.03
5	6	0.10	0.19	0.23	0.04	0.00	-0.04	-0.05	0.00	0.00
6	6	-0.06	-0.26	-0.27	-0.08	0.13	0.01	0.01	0.00	-0.02
7	1	0.05	0.14	0.07	-0.18	0.21	-0.07	0.04	0.02	0.02
8	6	-0.08	-0.14	-0.48	0.07	0.06	-0.10	0.01	-0.01	-0.04
9	1	0.10	-0.02	0.17	0.17	0.16	-0.14	0.05	0.02	0.01
10	6	-0.04	-0.01	0.00	-0.05	0.08	-0.07	0.03	0.07	0.12
11	1	-0.01	0.01	0.02	-0.10	0.08	-0.08	0.02	0.07	0.12
12	6	-0.01	-0.02	-0.01	-0.03	0.11	-0.09	0.12	0.14	0.25
13	1	-0.01	0.00	-0.01	-0.05	0.13	-0.11	0.19	0.19	0.35
14	6	0.00	0.01	-0.03	0.03	0.11	-0.08	0.14	0.15	0.26
15	1	0.01	0.01	-0.01	0.05	0.14	-0.09	0.22	0.20	0.37
16	6	-0.03	0.00	-0.02	0.06	0.08	-0.05	0.06	0.08	0.14
17	1	-0.02	0.01	-0.01	0.10	0.09	-0.05	0.07	0.09	0.15
18	6	-0.03	0.03	0.01	0.02	-0.02	-0.01	-0.05	0.00	0.00
19	6	-0.03	0.01	0.05	-0.02	0.00	0.01	-0.05	0.01	0.02

```
    20   6     0.02  -0.01  -0.02    -0.04  -0.02   0.06    -0.05
0.02   0.04
    21   1     0.02   0.00   0.02    -0.07  -0.01   0.08    -0.05
0.02   0.06
    22   6    -0.01  -0.02  -0.01    -0.02  -0.06   0.08    -0.05
0.02   0.05
    23   1     0.00  -0.01  -0.01    -0.04  -0.07   0.12    -0.05
0.03   0.07
    24   6    -0.01   0.01  -0.02     0.02  -0.07   0.05    -0.05
0.01   0.02
    25   1    -0.01   0.01   0.00     0.03  -0.10   0.07    -0.05
0.01   0.03
    26   6     0.01  -0.01  -0.03     0.04  -0.06   0.01    -0.05
0.00   0.00
    27   1     0.01   0.00  -0.01     0.07  -0.07  -0.01    -0.05  -
0.01  -0.02
    28   6    -0.01  -0.02  -0.06     0.12  -0.13  -0.08     0.02  -
0.08  -0.14
    29   6    -0.04  -0.03  -0.02    -0.16   0.03   0.16     0.01  -
0.07  -0.12
    30   8    -0.03   0.02   0.02    -0.02  -0.14   0.10     0.01  -
0.10  -0.18
    31   8     0.00   0.01   0.02    -0.29   0.07   0.32     0.02  -
0.10  -0.17
    32   8     0.00   0.01   0.02     0.25  -0.25  -0.19     0.04  -
0.12  -0.21
    33   6     0.02   0.05   0.05     0.09   0.00  -0.04    -0.05  -
0.01  -0.01
    34   1    -0.01   0.17  -0.11     0.13  -0.01  -0.04    -0.01  -
0.01  -0.03
    35   1     0.01  -0.05   0.04     0.09   0.05  -0.03    -0.07
0.01   0.02
    36   1     0.01  -0.03   0.04     0.08  -0.03  -0.04    -0.08  -
0.03  -0.04
                      4                      5                      6
                      A                      A                      A
 Frequencies --    84.2318                98.7638
132.7046
 Red. masses --     5.4062                 5.5632
4.8458
 Frc consts  --     0.0226                 0.0320
0.0503
 IR Inten    --     0.7452                 1.4926
0.3450
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.04  -0.06  -0.06     0.01  -0.01   0.09     0.01
0.03   0.01
     2   6     0.03  -0.06  -0.07     0.04   0.01   0.17    -0.01
0.01  -0.03
     3   1     0.03  -0.06  -0.07     0.05   0.01   0.18     0.01
0.03   0.03
```

```
     4   6     0.03  -0.06  -0.08    -0.04  -0.06  -0.01    -0.02
0.01  -0.04
     5   6     0.00  -0.07  -0.11    -0.07  -0.12  -0.08     0.01
0.04   0.02
     6   6    -0.08  -0.03  -0.09     0.06   0.07   0.09     0.02  -
0.14   0.02
     7   1    -0.10  -0.05  -0.12     0.05   0.03   0.06     0.06  -
0.16   0.06
     8   6    -0.09  -0.04  -0.11     0.01   0.01  -0.01    -0.03  -
0.09   0.09
     9   1    -0.11  -0.07  -0.13     0.02   0.02   0.03    -0.07  -
0.13   0.11
    10   6     0.09  -0.03   0.00     0.03   0.02   0.14     0.06
0.09   0.09
    11   1     0.10  -0.03   0.02     0.08   0.06   0.23     0.10
0.12   0.17
    12   6     0.12  -0.01   0.05     0.00   0.00   0.06     0.05
0.08   0.06
    13   1     0.16   0.01   0.11     0.02   0.03   0.09     0.09
0.12   0.12
    14   6     0.10  -0.02   0.03    -0.06  -0.05  -0.05    -0.03
0.02  -0.08
    15   1     0.12  -0.01   0.07    -0.09  -0.07  -0.12    -0.07
0.00  -0.13
    16   6     0.05  -0.05  -0.04    -0.08  -0.08  -0.09    -0.06  -
0.01  -0.12
    17   1     0.04  -0.06  -0.06    -0.12  -0.13  -0.17    -0.11  -
0.06  -0.21
    18   6     0.01  -0.05  -0.07    -0.03  -0.05  -0.02     0.00
0.04   0.04
    19   6     0.02  -0.05  -0.07     0.02   0.01   0.09    -0.01
0.00  -0.05
    20   6     0.05   0.04   0.07     0.05   0.06   0.14    -0.01  -
0.06  -0.19
    21   1     0.07   0.04   0.09     0.08   0.11   0.25    -0.02  -
0.12  -0.32
    22   6     0.06   0.14   0.24     0.02   0.04   0.02    -0.01  -
0.02  -0.14
    23   1     0.08   0.22   0.38     0.04   0.08   0.04    -0.02  -
0.07  -0.24
    24   6     0.04   0.13   0.23    -0.03  -0.04  -0.14     0.01
0.09   0.09
    25   1     0.05   0.21   0.36    -0.06  -0.06  -0.25     0.02
0.13   0.18
    26   6     0.02   0.03   0.06    -0.06  -0.08  -0.15     0.01
0.12   0.16
    27   1     0.00   0.03   0.05    -0.10  -0.13  -0.27     0.01
0.19   0.30
    28   6    -0.09   0.02  -0.02     0.02   0.03  -0.06    -0.06  -
0.07  -0.01
    29   6    -0.08   0.03   0.00     0.05   0.10   0.06     0.06  -
0.04   0.06
```

```
    30   8    -0.08   0.06   0.04     0.04   0.10  -0.01     0.00  -
0.02   0.03
    31   8    -0.08   0.06   0.04     0.11   0.14   0.09     0.11
0.04   0.14
    32   8    -0.12   0.05   0.01    -0.03   0.00  -0.18    -0.11  -
0.11  -0.15
    33   6     0.00  -0.08  -0.12    -0.08  -0.14  -0.11     0.01
0.01  -0.02
    34   1     0.03  -0.08  -0.14     0.00  -0.14  -0.15    -0.16
0.05  -0.02
    35   1     0.00  -0.07  -0.11    -0.10  -0.11  -0.06     0.05  -
0.10  -0.14
    36   1    -0.01  -0.11  -0.13    -0.14  -0.19  -0.16     0.11
0.05   0.08
                     7                      8                      9
                     A                      A                      A
 Frequencies --   143.2514               152.0717
178.9941
 Red. masses --     5.1065                 7.7442
3.5679
 Frc consts  --     0.0617                 0.1055
0.0674
 IR Inten    --     0.1513                 3.0114
0.2289
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.04  -0.01  -0.07     0.11   0.05   0.10    -0.01  -
0.01   0.04
     2   6    -0.02  -0.01  -0.06     0.09   0.04   0.08     0.02
0.00   0.10
     3   1     0.00   0.01  -0.01     0.11   0.06   0.12     0.00  -
0.02   0.06
     4   6     0.02   0.03   0.02     0.11   0.05   0.10     0.01  -
0.01   0.05
     5   6     0.00   0.04   0.01     0.09   0.04   0.08    -0.02  -
0.07  -0.01
     6   6     0.04  -0.17  -0.01    -0.13   0.04   0.14     0.01
0.06   0.05
     7   1     0.08  -0.19   0.03    -0.11  -0.01   0.13    -0.01
0.04   0.01
     8   6    -0.01  -0.12   0.07    -0.14   0.05   0.17     0.01
0.02  -0.03
     9   1    -0.06  -0.17   0.09    -0.16   0.03   0.12     0.03
0.04  -0.02
    10   6    -0.11  -0.06  -0.18     0.05   0.01   0.01    -0.08  -
0.02  -0.05
    11   1    -0.20  -0.12  -0.31     0.05   0.00   0.01    -0.15  -
0.04  -0.09
    12   6    -0.06  -0.03  -0.11    -0.05  -0.06  -0.12    -0.07
0.00  -0.08
    13   1    -0.12  -0.07  -0.19    -0.12  -0.11  -0.23    -0.13  -
0.02  -0.16
```

```
    14    6     0.07   0.07   0.10    -0.03  -0.05  -0.10     0.03
0.05   0.03
    15    1     0.15   0.12   0.21    -0.10  -0.09  -0.20     0.07
0.08   0.06
    16    6     0.11   0.10   0.15     0.06   0.02   0.03     0.07
0.04   0.08
    17    1     0.20   0.16   0.28     0.07   0.02   0.05     0.15
0.07   0.13
    18    6    -0.01   0.01  -0.05     0.09   0.01   0.01    -0.01  -
0.01   0.06
    19    6    -0.01   0.03  -0.01     0.10   0.02   0.03     0.01  -
0.02   0.04
    20    6     0.01   0.09   0.06     0.12   0.05   0.06     0.03  -
0.04  -0.10
    21    1     0.04   0.12   0.13     0.14   0.08   0.10     0.06  -
0.09  -0.18
    22    6     0.00   0.10   0.04     0.11   0.06   0.03     0.01
0.00  -0.11
    23    1     0.01   0.14   0.10     0.12   0.08   0.05     0.02  -
0.03  -0.22
    24    6    -0.02   0.04  -0.08     0.09   0.02  -0.05    -0.01
0.08   0.05
    25    1    -0.03   0.02  -0.13     0.09   0.01  -0.09    -0.02
0.13   0.10
    26    6    -0.03   0.00  -0.12     0.08   0.00  -0.05    -0.03
0.07   0.12
    27    1    -0.05  -0.03  -0.19     0.07  -0.02  -0.09    -0.07
0.12   0.20
    28    6    -0.05  -0.06   0.01    -0.17  -0.02  -0.02     0.02
0.03   0.01
    29    6     0.09  -0.04   0.06    -0.13  -0.03  -0.01    -0.01
0.03   0.02
    30    8     0.03   0.00   0.05    -0.16  -0.03  -0.06     0.01
0.09   0.12
    31    8     0.15   0.06   0.16    -0.11  -0.12  -0.16    -0.02  -
0.06  -0.10
    32    8    -0.11  -0.07  -0.07    -0.19  -0.12  -0.24     0.03
0.00  -0.05
    33    6    -0.05   0.02  -0.02     0.10   0.05   0.10    -0.02  -
0.17  -0.16
    34    1    -0.01   0.03  -0.05     0.22   0.02   0.10     0.23  -
0.12  -0.33
    35    1    -0.08   0.00   0.04     0.08   0.14   0.18    -0.08  -
0.09   0.01
    36    1    -0.09   0.00  -0.06     0.04   0.02   0.04    -0.18  -
0.39  -0.29
                     10                     11                     12
                      A                      A                      A
 Frequencies --    182.5568               213.9995
240.5759
 Red. masses --      9.0544                 1.3021
3.4289
```

This journal is © The Royal Society of Chemistry 2014

```
 Frc consts  --     0.1778                  0.0351
0.1169
 IR Inten    --     3.2608                  0.4413
0.2048
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.02   0.00  -0.06     0.02   0.00   0.02     0.04
0.09  -0.02
     2   6    -0.04   0.00  -0.09     0.02   0.01   0.01     0.00
0.09  -0.05
     3   1    -0.02   0.01  -0.07     0.02   0.01   0.01     0.00
0.10  -0.03
     4   6    -0.04   0.00  -0.06     0.02   0.00   0.02     0.01
0.11   0.02
     5   6     0.00   0.05  -0.01     0.01   0.00   0.00     0.03
0.12   0.01
     6   6     0.02  -0.05  -0.08    -0.01   0.02   0.01    -0.01  -
0.03  -0.02
     7   1     0.00  -0.09  -0.13    -0.01   0.02   0.01     0.01  -
0.01   0.01
     8   6     0.04  -0.02  -0.02     0.00   0.02   0.00     0.00
0.02   0.04
     9   1     0.01  -0.04  -0.07     0.00   0.02   0.00    -0.01
0.01   0.06
    10   6     0.04   0.00   0.01     0.00  -0.01  -0.01     0.09  -
0.04  -0.01
    11   1     0.08   0.01   0.03    -0.02  -0.01  -0.03     0.19  -
0.07  -0.06
    12   6     0.05   0.00   0.07    -0.01  -0.01  -0.03     0.02  -
0.13   0.04
    13   1     0.11   0.01   0.14    -0.03  -0.02  -0.05     0.04  -
0.21   0.04
    14   6    -0.02  -0.03   0.00     0.02   0.01   0.00    -0.06  -
0.12   0.06
    15   1    -0.03  -0.04   0.01     0.02   0.01   0.00    -0.12  -
0.18   0.08
    16   6    -0.07  -0.03  -0.05     0.03   0.01   0.02    -0.08
0.02   0.07
    17   1    -0.12  -0.04  -0.08     0.04   0.01   0.03    -0.16
0.05   0.12
    18   6    -0.02   0.01  -0.05     0.02   0.01   0.00     0.03
0.09   0.01
    19   6    -0.04   0.01  -0.04     0.01   0.01   0.00    -0.01
0.09  -0.01
    20   6    -0.06   0.01   0.05     0.00  -0.01   0.00    -0.09
0.00   0.03
    21   1    -0.10   0.04   0.10    -0.02  -0.01   0.00    -0.19
0.01   0.03
    22   6    -0.04  -0.02   0.09     0.01  -0.03   0.01    -0.05  -
0.10   0.05
    23   1    -0.05  -0.01   0.16     0.00  -0.04   0.00    -0.09  -
0.15   0.06
```

```
    24   6    -0.02  -0.07  -0.01     0.02  -0.03   0.01     0.02  -
0.10   0.03
    25   1    -0.01  -0.10  -0.02     0.03  -0.03   0.02     0.05  -
0.18   0.03
    26   6     0.00  -0.05  -0.07     0.03  -0.01   0.01     0.08  -
0.01   0.02
    27   1     0.05  -0.08  -0.11     0.05  -0.01   0.02     0.16  -
0.02   0.01
    28   6     0.04   0.05   0.07     0.00   0.01   0.00    -0.01
0.01   0.01
    29   6     0.03   0.01   0.05    -0.01   0.01   0.00     0.01
0.00  -0.01
    30   8     0.07   0.27   0.48    -0.01   0.00  -0.01     0.00  -
0.01  -0.01
    31   8     0.00  -0.18  -0.20    -0.01   0.00  -0.01     0.00
0.01   0.02
    32   8     0.04  -0.09  -0.22     0.00   0.01  -0.01     0.00  -
0.01  -0.02
    33   6     0.00   0.13   0.10    -0.12  -0.03  -0.04     0.01  -
0.03  -0.21
    34   1    -0.20   0.09   0.22    -0.69   0.09   0.01     0.19
0.08  -0.45
    35   1     0.04   0.07  -0.03    -0.01  -0.41  -0.39    -0.05  -
0.03  -0.09
    36   1     0.12   0.29   0.20     0.20   0.23   0.23    -0.12  -
0.27  -0.32
                     13                    14                    15
                      A                     A                     A
 Frequencies --   278.6623              328.3908
335.0386
 Red. masses --     4.2142                4.4144
2.3460
 Frc consts  --     0.1928                0.2805
0.1552
 IR Inten    --     6.2202                0.0678
0.6744
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.07  -0.05  -0.12    -0.01   0.05  -0.03     0.00
0.04   0.01
     2   6     0.02   0.00  -0.01     0.08   0.12   0.22    -0.03
0.00   0.01
     3   1     0.02   0.00   0.00     0.12   0.15   0.29    -0.09
0.01   0.02
     4   6    -0.07  -0.05  -0.12    -0.06   0.00  -0.14    -0.01
0.06   0.02
     5   6     0.02   0.00   0.00    -0.06  -0.06  -0.21     0.00
0.00   0.00
     6   6    -0.02   0.01   0.00     0.02   0.08   0.17     0.00
0.00   0.00
     7   1    -0.02  -0.01  -0.01    -0.03   0.01   0.08     0.00
0.01   0.01
```

```
     8   6    -0.01   0.00   0.01    -0.02  -0.01   0.02     0.00
0.01   0.00
     9   1    -0.02   0.00  -0.02     0.03   0.04   0.09     0.00
0.01   0.01
    10   6    -0.06  -0.08  -0.13    -0.03  -0.06  -0.11     0.01
0.01   0.02
    11   1    -0.08  -0.10  -0.18    -0.01  -0.10  -0.20     0.05
0.00   0.00
    12   6     0.07   0.01   0.07     0.00  -0.07   0.00    -0.03  -
0.04   0.02
    13   1     0.15   0.06   0.19     0.01  -0.09   0.00    -0.04  -
0.08   0.00
    14   6     0.07   0.01   0.09     0.07  -0.01   0.12    -0.05  -
0.03   0.04
    15   1     0.15   0.07   0.22     0.15   0.04   0.27    -0.08  -
0.06   0.04
    16   6    -0.06  -0.06  -0.10    -0.05  -0.02  -0.04    -0.04
0.03   0.06
    17   1    -0.10  -0.07  -0.14    -0.12  -0.01  -0.02    -0.06
0.04   0.07
    18   6     0.03   0.07   0.16    -0.01   0.00  -0.13    -0.04  -
0.07  -0.02
    19   6     0.03   0.07   0.16     0.01   0.06  -0.03    -0.02  -
0.06  -0.01
    20   6     0.05   0.09   0.15    -0.04  -0.04  -0.09     0.01  -
0.01  -0.03
    21   1     0.08   0.12   0.21    -0.12  -0.06  -0.15     0.07  -
0.02  -0.04
    22   6     0.03  -0.02  -0.11    -0.01  -0.07   0.00    -0.01
0.07   0.00
    23   1     0.02  -0.10  -0.27    -0.03  -0.10   0.00     0.02
0.13   0.04
    24   6     0.02  -0.03  -0.13     0.02  -0.01   0.13    -0.05
0.06  -0.02
    25   1     0.00  -0.11  -0.31     0.04   0.04   0.27    -0.07
0.12   0.01
    26   6     0.03   0.07   0.13     0.03  -0.02  -0.04    -0.08  -
0.02  -0.05
    27   1     0.02   0.10   0.18     0.10  -0.04  -0.06    -0.11  -
0.02  -0.05
    28   6    -0.03   0.00   0.00     0.00  -0.02   0.02     0.00
0.00   0.00
    29   6    -0.03   0.00   0.00    -0.01   0.00   0.07     0.00
0.00   0.00
    30   8    -0.02   0.00   0.00    -0.01  -0.02  -0.02     0.00
0.00   0.00
    31   8    -0.06  -0.01   0.00     0.05  -0.03   0.00     0.02
0.00  -0.01
    32   8    -0.06   0.01  -0.01    -0.03  -0.01   0.01     0.03  -
0.01   0.01
    33   6     0.12  -0.03  -0.03     0.03   0.11   0.02     0.24  -
0.04  -0.05
```

```
    34   1    -0.04   0.00  -0.02     0.02  -0.05   0.26    -0.08
0.01  -0.01
    35   1     0.20  -0.09  -0.22     0.06   0.27  -0.01     0.42  -
0.13  -0.45
    36   1     0.28  -0.02   0.11     0.08   0.28   0.06     0.56  -
0.03   0.25
                     16                    17                    18
                      A                     A                     A
 Frequencies --   370.4812              395.1301
414.0595
 Red. masses --     4.2823                8.1841
5.5451
 Frc consts  --     0.3463                0.7528
0.5601
 IR Inten    --     1.3711                1.4895
3.5465
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.08   0.02   0.01    -0.05   0.06   0.02     0.04  -
0.04  -0.01
     2   6     0.00  -0.01   0.03     0.00   0.05  -0.02     0.00  -
0.04   0.03
     3   1     0.00  -0.01   0.04     0.00   0.07   0.02     0.01  -
0.04   0.01
     4   6     0.06  -0.01  -0.03    -0.08   0.04  -0.01     0.08
0.00   0.05
     5   6    -0.05  -0.05  -0.14    -0.06  -0.10  -0.12     0.06
0.11   0.14
     6   6     0.02   0.00   0.00     0.14  -0.03  -0.11     0.09
0.10   0.14
     7   1    -0.01  -0.04  -0.06     0.13  -0.12  -0.17     0.13
0.19   0.24
     8   6     0.01  -0.04  -0.06     0.14  -0.09  -0.08     0.09
0.00   0.00
     9   1     0.03  -0.03  -0.05     0.18  -0.06  -0.08     0.15
0.06   0.00
    10   6     0.17   0.01   0.08    -0.03   0.09   0.10     0.02  -
0.08  -0.09
    11   1     0.27   0.05   0.17     0.04   0.12   0.17    -0.06  -
0.11  -0.17
    12   6     0.05  -0.08  -0.13    -0.15   0.00   0.02     0.14
0.01   0.00
    13   1    -0.03  -0.12  -0.24    -0.18  -0.08  -0.03     0.16
0.07   0.05
    14   6     0.07  -0.07  -0.09    -0.15   0.02   0.07     0.11  -
0.02  -0.06
    15   1     0.03  -0.11  -0.13    -0.16   0.02   0.05     0.09  -
0.04  -0.07
    16   6     0.17   0.05   0.07    -0.07   0.07   0.14     0.04  -
0.04  -0.12
    17   1     0.24   0.10   0.18    -0.05   0.12   0.24     0.01  -
0.10  -0.22
```

```
    18    6    -0.08    0.01    0.00     0.05   -0.02   -0.04     -0.03
0.04   0.08
    19    6    -0.06    0.03    0.04     0.07    0.01    0.00     -0.06
0.00   0.02
    20    6    -0.10    0.05    0.14     0.09    0.01    0.01     -0.11  -
0.05  -0.10
    21    1    -0.11    0.11    0.25     0.09    0.02    0.02     -0.12  -
0.12  -0.24
    22    6    -0.14   -0.04   -0.08     0.12   -0.04   -0.04     -0.12
0.07   0.08
    23    1    -0.13   -0.07   -0.20     0.10   -0.08   -0.07     -0.10
0.12   0.15
    24    6    -0.14   -0.02   -0.03     0.12   -0.02    0.02     -0.11
0.03   0.01
    25    1    -0.14   -0.06   -0.08     0.11    0.01    0.03     -0.10
0.01   0.02
    26    6    -0.10    0.09    0.13     0.09   -0.02    0.03     -0.10  -
0.02  -0.12
    27    1    -0.09    0.15    0.25     0.12   -0.01    0.05     -0.13  -
0.09  -0.26
    28    6     0.01   -0.03   -0.02     0.09   -0.04   -0.07      0.05  -
0.02  -0.03
    29    6     0.00   -0.01    0.01     0.07   -0.05   -0.05      0.06
0.00   0.07
    30    8     0.02    0.00    0.00     0.23    0.00    0.00      0.14  -
0.03  -0.02
    31    8    -0.01   -0.01    0.01    -0.28   -0.11    0.11     -0.14  -
0.12   0.04
    32    8    -0.04    0.01    0.01    -0.28    0.15   -0.05     -0.18
0.10  -0.03
    33    6     0.03    0.07    0.01     0.02    0.00    0.03      0.01
0.00  -0.03
    34    1    -0.01   -0.04    0.18     0.01   -0.12    0.20     -0.02
0.13  -0.20
    35    1     0.06    0.16   -0.04     0.04    0.11    0.01      0.01  -
0.13  -0.06
    36    1     0.09    0.19    0.06     0.07    0.11    0.07      0.00  -
0.11  -0.03
                     19                     20                     21
                      A                      A                      A
 Frequencies --   419.3147               427.8898
484.4570
 Red. masses --     4.7719                 6.2764
3.2193
 Frc consts  --     0.4943                 0.6771
0.4452
 IR Inten    --     0.3762                 2.4951
7.1744
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.09   0.14  -0.11     0.04   0.02   0.09     -0.08  -
0.05  -0.13
```

```
     2   6     0.02   0.00   0.01     0.03   0.03   0.11     0.01
0.00   0.00
     3   1    -0.21   0.04   0.06     0.03   0.04   0.13     0.00
0.00   0.00
     4   6    -0.04   0.16  -0.04     0.02  -0.05  -0.04    -0.10  -
0.06  -0.14
     5   6    -0.03   0.02   0.02     0.00  -0.02  -0.02     0.00
0.00   0.00
     6   6     0.00   0.01   0.01     0.01  -0.19  -0.26    -0.01
0.00   0.00
     7   1     0.00   0.02   0.02     0.09  -0.34  -0.23    -0.02  -
0.01  -0.01
     8   6     0.00   0.00   0.01     0.03   0.16   0.32    -0.01
0.00   0.01
     9   1     0.00   0.01   0.01    -0.07   0.06   0.43    -0.02  -
0.01  -0.01
    10   6     0.14   0.05  -0.16    -0.01  -0.05  -0.02     0.08
0.03   0.08
    11   1     0.19   0.01  -0.22    -0.04  -0.08  -0.08     0.25
0.14   0.33
    12   6     0.12  -0.02  -0.05     0.01  -0.04  -0.04    -0.01  -
0.03  -0.06
    13   1     0.18  -0.13  -0.01    -0.05  -0.03  -0.10     0.02
0.00  -0.01
    14   6    -0.04   0.02   0.02     0.11  -0.01   0.03    -0.01  -
0.02  -0.04
    15   1    -0.10  -0.06   0.11     0.16   0.03   0.09     0.04
0.01   0.05
    16   6    -0.11   0.13  -0.03     0.03  -0.05  -0.06     0.06
0.05   0.07
    17   1    -0.20   0.14  -0.02     0.01  -0.07  -0.10     0.24
0.17   0.32
    18   6    -0.08  -0.13   0.08    -0.04  -0.04  -0.03     0.01
0.08   0.18
    19   6     0.07  -0.17   0.07     0.01   0.02   0.09     0.02
0.07   0.16
    20   6     0.15  -0.12   0.05    -0.02  -0.04  -0.01     0.01  -
0.05  -0.11
    21   1     0.24  -0.13   0.06    -0.03  -0.07  -0.07    -0.01  -
0.20  -0.41
    22   6     0.10  -0.02  -0.01    -0.04  -0.02  -0.03     0.03
0.02   0.06
    23   1     0.18   0.07  -0.07    -0.03  -0.02  -0.10     0.02  -
0.01  -0.01
    24   6    -0.07   0.00   0.01    -0.07   0.04   0.07     0.02
0.02   0.04
    25   1    -0.13   0.11  -0.04    -0.06   0.08   0.14     0.00  -
0.01  -0.06
    26   6    -0.14  -0.09   0.07    -0.07  -0.02  -0.04     0.00  -
0.07  -0.09
    27   1    -0.22  -0.08   0.08    -0.08  -0.04  -0.07    -0.03  -
0.22  -0.40
```

```
    28   6     0.00   0.00   0.00     0.04   0.16   0.11    -0.01
0.00   0.01
    29   6     0.00   0.00   0.00     0.00  -0.03  -0.18    -0.02
0.00   0.00
    30   8     0.00   0.00   0.00     0.03   0.04  -0.05    -0.03
0.00   0.00
    31   8     0.00   0.00   0.00    -0.16   0.06   0.06     0.01
0.01  -0.01
    32   8     0.00   0.00   0.00     0.08   0.03  -0.11     0.01  -
0.01   0.00
    33   6    -0.13   0.03   0.03     0.01   0.00   0.01     0.00
0.00   0.00
    34   1    -0.11   0.03   0.03     0.01  -0.02   0.04    -0.02
0.00   0.01
    35   1    -0.21  -0.03   0.18     0.01   0.01   0.02    -0.01  -
0.02   0.00
    36   1    -0.25   0.11  -0.09     0.00   0.01   0.01     0.00
0.02   0.00
                     22                    23                    24
                      A                     A                     A
 Frequencies --   523.9592              528.8031
550.9908
 Red. masses --     4.2540                3.8309
3.5394
 Frc consts  --     0.6881                0.6312
0.6331
 IR Inten    --     7.1754                0.0120
36.9229
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.04  -0.11  -0.04    -0.11  -0.03  -0.12     0.10
0.02   0.16
     2   6     0.00  -0.13   0.08    -0.06  -0.01   0.03    -0.02  -
0.08  -0.07
     3   1     0.01  -0.13   0.08    -0.11   0.00   0.03    -0.05  -
0.14  -0.20
     4   6    -0.02  -0.09  -0.11     0.10   0.05   0.06     0.10
0.02   0.09
     5   6     0.03   0.21   0.00     0.07   0.02  -0.03    -0.04
0.03  -0.13
     6   6     0.01   0.02   0.06    -0.01   0.00   0.00    -0.02
0.00  -0.06
     7   1     0.05   0.06   0.13    -0.02  -0.01  -0.02    -0.08  -
0.06  -0.17
     8   6     0.00   0.04   0.07     0.01   0.01   0.01     0.02  -
0.03  -0.06
     9   1    -0.01   0.03   0.08     0.02   0.02   0.02     0.04  -
0.01  -0.17
    10   6    -0.04   0.03   0.07    -0.07  -0.03  -0.06    -0.04
0.02   0.00
    11   1     0.02   0.10   0.24    -0.01  -0.03  -0.04    -0.21  -
0.07  -0.20
```

12	6	-0.09	0.01	0.00	0.06	0.03	0.15	-0.06	0.02	0.02
13	1	-0.06	0.05	0.04	0.19	0.15	0.35	-0.16	-0.05	-0.13
14	6	-0.01	0.00	0.00	-0.07	-0.11	-0.13	0.02	0.02	0.06
15	1	0.09	0.09	0.03	-0.18	-0.17	-0.32	0.00	0.03	-0.07
16	6	0.04	-0.07	0.04	0.08	0.02	0.08	-0.01	-0.09	-0.03
17	1	0.17	-0.01	0.18	0.05	0.04	0.12	-0.15	-0.21	-0.25
18	6	-0.07	-0.05	-0.06	0.01	-0.09	-0.10	-0.04	0.05	0.12
19	6	-0.02	-0.12	-0.09	-0.03	0.02	0.15	0.02	0.05	0.16
20	6	0.08	-0.01	0.01	0.01	0.05	0.08	0.04	-0.01	-0.02
21	1	0.13	0.07	0.18	0.07	0.03	0.05	0.02	-0.12	-0.26
22	6	0.09	-0.01	0.01	-0.01	-0.04	-0.16	0.06	-0.01	0.00
23	1	0.11	0.06	0.11	-0.04	-0.16	-0.37	0.05	-0.08	-0.17
24	6	0.01	-0.04	-0.04	0.05	0.10	0.13	-0.01	0.01	0.06
25	1	-0.03	0.05	-0.05	0.06	0.20	0.33	-0.05	0.02	-0.07
26	6	-0.03	-0.05	0.09	0.01	-0.05	-0.08	-0.05	-0.08	-0.01
27	1	-0.04	0.03	0.25	-0.05	-0.05	-0.08	-0.06	-0.20	-0.26
28	6	0.01	0.04	0.03	0.00	0.00	0.00	0.00	-0.07	-0.03
29	6	0.02	0.01	0.03	-0.01	0.00	0.01	-0.03	-0.01	-0.02
30	8	0.02	0.00	-0.02	0.00	0.00	0.00	-0.01	-0.01	0.03
31	8	-0.02	-0.02	0.01	0.00	0.00	0.00	0.04	0.03	-0.02
32	8	0.01	0.02	-0.02	0.00	0.00	0.00	-0.04	-0.03	0.03
33	6	0.00	0.24	-0.17	-0.01	0.04	-0.03	0.01	0.16	-0.10
34	1	0.00	0.36	-0.35	-0.04	0.05	-0.03	0.03	0.08	0.01
35	1	-0.03	0.13	-0.17	-0.05	-0.02	0.03	0.03	0.25	-0.12
36	1	-0.03	0.12	-0.20	-0.06	0.10	-0.07	0.03	0.21	-0.09

25	26	27
A	A	A

```
 Frequencies --   567.7313                586.0745
604.3077
 Red. masses --     4.8003                  3.7527
4.7700
 Frc consts  --     0.9116                  0.7595
1.0263
 IR Inten    --     1.0784                  4.0522
9.2599
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.07  -0.16  -0.03     0.00  -0.03  -0.03     -0.05
0.01  -0.02
     2   6     0.22  -0.04  -0.06     0.06   0.00   0.07      0.02
0.07   0.05
     3   1     0.40  -0.06  -0.07     0.09   0.01   0.09      0.00
0.06   0.03
     4   6    -0.10  -0.07   0.10     0.05   0.03   0.08      0.02
0.01  -0.01
     5   6    -0.16   0.04   0.08    -0.07  -0.06  -0.12      0.00  -
0.03  -0.05
     6   6    -0.04   0.00  -0.01     0.08  -0.05   0.03     -0.15
0.04  -0.13
     7   1    -0.05   0.07   0.01     0.13  -0.24   0.00     -0.34
0.16  -0.31
     8   6     0.04   0.02   0.02    -0.08  -0.07   0.01      0.17
0.14   0.04
     9   1     0.03   0.02  -0.07    -0.18  -0.16   0.07      0.34
0.30   0.02
    10   6     0.03  -0.01  -0.05    -0.06  -0.03  -0.10     -0.06  -
0.03  -0.03
    11   1    -0.11   0.05   0.07    -0.12  -0.05  -0.15     -0.03  -
0.04  -0.03
    12   6     0.09   0.10  -0.06     0.08   0.07   0.11      0.02
0.01   0.08
    13   1     0.16   0.06   0.02     0.17   0.10   0.24      0.07
0.10   0.17
    14   6    -0.12   0.12  -0.03    -0.10  -0.04  -0.10     -0.01  -
0.06  -0.07
    15   1    -0.17   0.06  -0.03    -0.22  -0.12  -0.29     -0.04  -
0.07  -0.15
    16   6    -0.04   0.03   0.06     0.06   0.03   0.10      0.06
0.02   0.04
    17   1     0.13   0.00   0.00     0.04   0.00   0.04      0.06
0.04   0.09
    18   6    -0.10   0.08  -0.10    -0.02   0.07   0.08      0.00
0.00   0.01
    19   6     0.13   0.12  -0.03     0.02   0.01  -0.04      0.02  -
0.02  -0.04
    20   6     0.05   0.01   0.06     0.00  -0.04  -0.10      0.01  -
0.07  -0.06
    21   1    -0.14   0.03   0.08    -0.04  -0.07  -0.17      0.01  -
0.06  -0.04
```

```
    22   6     0.04  -0.14  -0.03     0.03   0.04   0.13     0.01
0.04   0.09
    23   1     0.08  -0.13  -0.15     0.05   0.10   0.25     0.05
0.14   0.23
    24   6    -0.12  -0.05   0.13    -0.03  -0.08  -0.10    -0.04  -
0.05  -0.09
    25   1    -0.13   0.05   0.24    -0.06  -0.16  -0.30    -0.05  -
0.09  -0.19
    26   6    -0.07  -0.01  -0.06    -0.01   0.04   0.09    -0.01
0.05   0.08
    27   1     0.11  -0.01  -0.03     0.02   0.01   0.03    -0.01
0.07   0.13
    28   6     0.02   0.00   0.03    -0.05   0.05   0.01     0.16  -
0.06   0.07
    29   6    -0.03  -0.01   0.01     0.05   0.02  -0.05    -0.17  -
0.10   0.03
    30   8    -0.01  -0.02   0.00     0.00   0.05  -0.03    -0.01  -
0.10   0.05
    31   8     0.03   0.01   0.00    -0.08   0.00   0.02     0.16
0.04  -0.01
    32   8    -0.03   0.01  -0.01     0.08  -0.02   0.00    -0.15
0.06  -0.05
    33   6     0.04  -0.02   0.00     0.00   0.03  -0.03     0.00
0.00   0.00
    34   1     0.11   0.01  -0.07     0.02  -0.08   0.13     0.00  -
0.03   0.03
    35   1     0.16   0.09  -0.20     0.04   0.17  -0.06    -0.01
0.01   0.02
    36   1     0.17  -0.26   0.15     0.06   0.10   0.02    -0.02
0.03  -0.02
                     28                    29                    30
                      A                     A                     A
 Frequencies --   619.9953              626.3140
665.1737
 Red. masses --     7.6150                7.6855
6.0501
 Frc consts  --     1.7246                1.7763
1.5772
 IR Inten    --     3.8215               16.7768
1.2760
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.09  -0.01   0.06     0.05   0.00  -0.09     0.15  -
0.05  -0.07
     2   6    -0.08   0.04   0.06     0.11  -0.01   0.02    -0.01  -
0.21   0.13
     3   1    -0.06   0.06   0.10     0.14   0.02   0.09     0.02  -
0.17   0.23
     4   6    -0.09   0.04   0.05     0.07  -0.06  -0.08     0.03  -
0.04   0.00
     5   6    -0.13   0.03   0.05     0.14   0.00   0.00     0.00  -
0.01  -0.01
```

```
     6   6    -0.03   0.05  -0.01    -0.01   0.05   0.00    -0.06  -
0.02   0.00
     7   1     0.16   0.00   0.19     0.13  -0.09   0.10    -0.07
0.00   0.01
     8   6    -0.02   0.01   0.05    -0.02   0.00   0.04     0.06
0.00   0.05
     9   1     0.19   0.20   0.07     0.11   0.12  -0.06     0.10
0.04   0.01
    10   6    -0.01  -0.18   0.08     0.00   0.17  -0.08     0.14
0.16  -0.17
    11   1    -0.02  -0.18   0.09     0.07   0.19  -0.02     0.08
0.17  -0.18
    12   6     0.13  -0.04  -0.05    -0.12   0.04   0.06     0.06
0.05  -0.06
    13   1     0.07   0.14  -0.05    -0.02  -0.09   0.13     0.16  -
0.25  -0.04
    14   6     0.12  -0.03  -0.09    -0.11   0.01   0.06    -0.15
0.08   0.07
    15   1     0.04  -0.14   0.01     0.00   0.14   0.00    -0.17
0.08   0.02
    16   6     0.03   0.16  -0.08    -0.01  -0.16   0.08    -0.06  -
0.10   0.10
    17   1     0.05   0.16  -0.08     0.03  -0.12   0.16    -0.01  -
0.14   0.03
    18   6    -0.10  -0.01  -0.02     0.12   0.00  -0.01    -0.04  -
0.04   0.02
    19   6    -0.07   0.03  -0.05     0.11  -0.05   0.01    -0.18
0.01   0.01
    20   6     0.03   0.14  -0.08    -0.02  -0.20   0.09    -0.14
0.22  -0.10
    21   1     0.01   0.17  -0.03     0.00  -0.19   0.10    -0.09
0.20  -0.13
    22   6     0.14  -0.01   0.00    -0.15   0.01   0.01    -0.06
0.08  -0.02
    23   1     0.06  -0.10   0.10    -0.04   0.17  -0.04    -0.24  -
0.17   0.07
    24   6     0.11  -0.04   0.00    -0.15   0.03  -0.01     0.19
0.02  -0.03
    25   1     0.04   0.11  -0.04    -0.07  -0.12   0.08     0.18
0.01  -0.08
    26   6    -0.01  -0.14   0.08     0.00   0.18  -0.09     0.06  -
0.13   0.07
    27   1     0.02  -0.11   0.14    -0.01   0.19  -0.07    -0.03  -
0.13   0.05
    28   6     0.01  -0.23   0.05    -0.01  -0.19   0.09     0.07  -
0.01   0.04
    29   6     0.03   0.15  -0.19     0.03   0.17  -0.15    -0.07
0.00  -0.02
    30   8     0.16   0.00   0.07     0.13   0.00   0.04     0.02  -
0.01   0.00
    31   8    -0.07   0.21  -0.12    -0.08   0.19  -0.12     0.01
0.05  -0.03
```

```
    32   8    -0.10  -0.19   0.11    -0.09  -0.20   0.10    -0.02
0.02  -0.02
    33   6    -0.01   0.00   0.00     0.01   0.00   0.00     0.00  -
0.06   0.03
    34   1     0.06   0.03  -0.06    -0.09   0.04  -0.03     0.00  -
0.09   0.08
    35   1     0.06   0.09  -0.12    -0.07  -0.15   0.11     0.00  -
0.03   0.04
    36   1     0.07  -0.16   0.09    -0.08   0.11  -0.09     0.01  -
0.03   0.04
                     31                     32                     33
                      A                      A                      A
 Frequencies --   710.2699               717.2183
733.7062
 Red. masses --     7.1816                 5.9960
6.6428
 Frc consts  --     2.1346                 1.8172
2.1069
 IR Inten    --    18.4900                 7.2490
7.5325
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.03   0.06  -0.04     0.00   0.11  -0.06    -0.01
0.00   0.00
     2   6     0.02   0.10  -0.02     0.00   0.14  -0.09     0.01
0.01  -0.03
     3   1    -0.03   0.03  -0.18     0.04   0.20   0.03     0.01  -
0.01  -0.06
     4   6     0.06  -0.04  -0.04     0.09  -0.02  -0.06     0.00
0.02   0.01
     5   6     0.00   0.00   0.02     0.02   0.03   0.05     0.02  -
0.01   0.00
     6   6     0.17   0.21  -0.15    -0.09  -0.13   0.10    -0.01  -
0.09  -0.11
     7   1     0.16   0.17  -0.19    -0.01   0.05   0.29    -0.21  -
0.34  -0.48
     8   6    -0.13   0.27  -0.14     0.06  -0.14   0.08     0.01  -
0.04  -0.04
     9   1    -0.11   0.27   0.04     0.09  -0.12   0.09    -0.13  -
0.15  -0.23
    10   6     0.00   0.11  -0.07    -0.02   0.15  -0.05    -0.01  -
0.02   0.03
    11   1     0.11   0.12  -0.06     0.14   0.12  -0.10    -0.03  -
0.03   0.00
    12   6    -0.07   0.00   0.05    -0.14  -0.01   0.09    -0.01  -
0.01   0.01
    13   1    -0.01  -0.03   0.12    -0.12  -0.02   0.11    -0.05
0.00  -0.04
    14   6     0.01  -0.05   0.00     0.08  -0.10  -0.01     0.01
0.00   0.01
    15   1     0.13   0.09  -0.07     0.23   0.08  -0.13    -0.03  -
0.03  -0.02
```

```
    16   6     0.06  -0.15   0.03     0.10  -0.17   0.00    -0.01
0.03  -0.01
    17   1     0.09  -0.11   0.10     0.06  -0.14   0.07    -0.06
0.01  -0.05
    18   6    -0.09   0.00   0.01    -0.10   0.02  -0.01    -0.02  -
0.02  -0.02
    19   6    -0.02   0.07  -0.04     0.02   0.11  -0.06    -0.01
0.02   0.02
    20   6     0.01   0.12  -0.06     0.05   0.12  -0.07     0.00
0.02  -0.02
    21   1    -0.08   0.16   0.00    -0.11   0.15  -0.04    -0.02
0.00  -0.07
    22   6     0.09  -0.04   0.00     0.15  -0.07   0.02     0.01
0.01   0.02
    23   1     0.06  -0.06   0.06     0.15  -0.06   0.04    -0.01  -
0.02   0.00
    24   6    -0.03  -0.04   0.02    -0.11  -0.07   0.04     0.00  -
0.01  -0.01
    25   1    -0.11   0.14   0.01    -0.22   0.15  -0.03    -0.02
0.01  -0.05
    26   6    -0.09  -0.12   0.06    -0.14  -0.11   0.07    -0.01  -
0.02   0.03
    27   1    -0.06  -0.10   0.11    -0.06  -0.10   0.11    -0.02  -
0.02   0.03
    28   6    -0.19   0.06   0.17     0.08  -0.06  -0.15     0.03
0.08   0.28
    29   6     0.20  -0.07  -0.04    -0.08   0.06   0.05     0.03
0.35   0.41
    30   8    -0.01  -0.09   0.03     0.01   0.06  -0.01     0.08  -
0.10  -0.17
    31   8     0.06  -0.11   0.10    -0.04   0.04  -0.06    -0.03  -
0.03  -0.14
    32   8    -0.07  -0.14   0.01     0.05   0.08   0.01    -0.02  -
0.06  -0.05
    33   6     0.00  -0.09   0.06     0.00  -0.10   0.08    -0.01  -
0.02   0.01
    34   1     0.00  -0.07   0.03    -0.01  -0.06   0.02    -0.02  -
0.02   0.02
    35   1    -0.01  -0.11   0.07    -0.01  -0.15   0.09    -0.01  -
0.01   0.02
    36   1     0.00  -0.11   0.06    -0.01  -0.14   0.08    -0.01
0.01   0.00
                     34                     35                     36
                      A                      A                      A
 Frequencies --   759.4859               763.8627
768.1991
 Red. masses --     5.6478                 2.9438
1.4820
 Frc consts  --     1.9194                 1.0120
0.5153
 IR Inten    --     8.2700                 0.9839
3.7664
```

This journal is © The Royal Society of Chemistry 2014

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.03	0.02	-0.04	0.12	0.08	0.17	0.02	0.02	0.03
2	6	0.00	0.00	-0.02	-0.01	0.00	0.00	-0.01	0.00	0.00
3	1	0.02	0.02	0.02	-0.02	-0.01	-0.03	-0.02	-0.01	-0.02
4	6	0.01	0.03	-0.01	-0.08	-0.06	-0.12	-0.06	-0.04	-0.07
5	6	0.01	-0.01	-0.01	0.00	0.00	0.00	-0.01	0.00	0.00
6	6	-0.06	0.03	0.15	0.00	-0.02	-0.03	0.00	-0.01	-0.01
7	1	0.01	0.09	0.27	0.00	0.02	-0.01	0.00	0.00	0.00
8	6	0.03	-0.14	-0.13	-0.01	0.02	0.02	0.00	0.00	0.00
9	1	-0.11	-0.26	-0.23	0.02	0.04	0.05	0.01	0.00	0.00
10	6	-0.02	0.01	0.04	-0.05	-0.03	-0.07	0.01	0.01	0.00
11	1	-0.04	-0.04	-0.07	-0.08	-0.05	-0.12	-0.16	-0.10	-0.26
12	6	-0.04	-0.01	0.04	0.03	0.02	0.05	0.04	0.02	0.05
13	1	-0.16	-0.03	-0.11	0.16	0.11	0.25	-0.16	-0.11	-0.24
14	6	0.05	-0.02	0.01	-0.06	-0.05	-0.09	0.00	0.00	0.00
15	1	-0.04	-0.08	-0.16	0.14	0.09	0.19	-0.17	-0.12	-0.26
16	6	0.02	0.03	-0.01	0.01	0.02	0.02	0.04	0.01	0.05
17	1	-0.12	-0.03	-0.12	0.28	0.21	0.41	-0.05	-0.05	-0.09
18	6	0.01	0.07	0.13	0.01	0.04	0.10	0.00	0.05	0.09
19	6	-0.01	-0.07	-0.17	-0.01	-0.08	-0.15	-0.01	-0.01	0.00
20	6	0.02	0.04	0.06	-0.01	0.03	0.07	0.00	-0.02	-0.02
21	1	0.01	0.07	0.13	0.01	0.04	0.09	0.05	0.16	0.35
22	6	0.01	-0.03	-0.05	-0.02	-0.01	-0.04	-0.01	-0.03	-0.07
23	1	0.00	-0.10	-0.21	-0.05	-0.12	-0.25	0.03	0.20	0.41
24	6	-0.01	0.04	0.09	0.02	0.05	0.08	0.01	-0.01	-0.02
25	1	-0.04	-0.05	-0.15	0.00	-0.11	-0.22	0.05	0.21	0.43

```
    26   6    -0.02  -0.03  -0.02     0.00  -0.02  -0.01     0.00  -
0.03  -0.07
    27   1    -0.04  -0.19  -0.35    -0.04  -0.20  -0.38     0.03
0.10   0.19
    28   6     0.10   0.16   0.38     0.00  -0.03  -0.06     0.00
0.00  -0.01
    29   6    -0.09  -0.13  -0.19     0.01   0.04   0.05     0.00
0.01   0.01
    30   8     0.04  -0.02  -0.03     0.01   0.00   0.00    -0.01
0.00   0.00
    31   8     0.00   0.08   0.02     0.00  -0.01  -0.01     0.00
0.00   0.00
    32   8     0.00  -0.01  -0.11     0.00   0.01   0.01     0.00
0.00   0.00
    33   6     0.00  -0.01   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    34   1    -0.01  -0.01   0.02    -0.01   0.00   0.00     0.00
0.00   0.01
    35   1     0.00  -0.03   0.02     0.00  -0.01   0.00     0.00
0.02   0.00
    36   1    -0.01   0.03  -0.01     0.01   0.02   0.00     0.00
0.00   0.00
                    37                    38                    39
                     A                     A                     A
 Frequencies --   771.9721              795.6399
834.0743
 Red. masses --     1.3749                3.2986
1.7938
 Frc consts  --     0.4827                1.2303
0.7353
 IR Inten    --    77.4549                1.1221
8.5780
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.03   0.01   0.04    -0.09  -0.06  -0.14    -0.01
0.02  -0.02
     2   6     0.00   0.00  -0.02     0.02  -0.01   0.08    -0.08
0.03   0.00
     3   1    -0.04  -0.04  -0.11     0.06   0.03   0.18    -0.29  -
0.05  -0.19
     4   6     0.04   0.03   0.05     0.09   0.07   0.13     0.01  -
0.02   0.04
     5   6    -0.01  -0.01  -0.02    -0.01  -0.03  -0.04    -0.12  -
0.01  -0.02
     6   6     0.00   0.00   0.02     0.02   0.00  -0.06    -0.04  -
0.05  -0.03
     7   1    -0.02  -0.06  -0.02    -0.08  -0.24  -0.31     0.15
0.45   0.47
     8   6     0.01  -0.03  -0.02    -0.01   0.06   0.06    -0.03
0.02  -0.01
     9   1    -0.02  -0.05  -0.06     0.03   0.09   0.09     0.07
0.08   0.33
```

This journal is © The Royal Society of Chemistry 2014

```
    10   6    -0.02  -0.02  -0.03     0.01   0.01   0.02     0.02
0.04  -0.04
    11   1     0.15   0.10   0.24     0.18   0.12   0.28     0.11
0.08   0.04
    12   6    -0.03  -0.02  -0.04    -0.04  -0.02  -0.06     0.02
0.00  -0.03
    13   1     0.24   0.16   0.35     0.04   0.03   0.06     0.08  -
0.02   0.04
    14   6    -0.03  -0.01  -0.03     0.04   0.02   0.05     0.02
0.00   0.00
    15   1     0.25   0.17   0.36    -0.01  -0.01  -0.01     0.03
0.02  -0.05
    16   6    -0.03  -0.02  -0.05    -0.01  -0.01  -0.02     0.02  -
0.07   0.03
    17   1     0.15   0.11   0.23    -0.16  -0.12  -0.24     0.03  -
0.12  -0.07
    18   6     0.00   0.02   0.04     0.02   0.10   0.17    -0.02
0.05  -0.01
    19   6     0.00   0.02   0.04    -0.01  -0.08  -0.18    -0.02  -
0.04   0.02
    20   6    -0.01  -0.01  -0.03     0.01   0.01   0.02     0.03  -
0.07   0.03
    21   1     0.02   0.10   0.19     0.03   0.19   0.38     0.09  -
0.06   0.06
    22   6    -0.01  -0.01  -0.03     0.00  -0.04  -0.08     0.02  -
0.01   0.00
    23   1     0.02   0.15   0.30     0.02   0.05   0.08     0.04
0.01  -0.03
    24   6     0.00  -0.02  -0.03    -0.01   0.03   0.07     0.04
0.02   0.00
    25   1     0.03   0.16   0.31    -0.02  -0.01  -0.02     0.07  -
0.06  -0.02
    26   6     0.00  -0.02  -0.03    -0.01  -0.02  -0.03     0.05
0.06  -0.03
    27   1     0.01   0.09   0.20    -0.03  -0.17  -0.33     0.11
0.04  -0.08
    28   6     0.01   0.02   0.05    -0.01  -0.06  -0.10     0.00
0.02   0.03
    29   6    -0.02  -0.01  -0.02     0.00   0.03   0.05     0.01
0.03   0.04
    30   8     0.00   0.00  -0.01    -0.01   0.01   0.01     0.04  -
0.02  -0.01
    31   8     0.00   0.01   0.00     0.01  -0.02  -0.01     0.00  -
0.01  -0.01
    32   8     0.00   0.00  -0.01     0.00   0.01   0.03     0.00
0.00  -0.01
    33   6     0.00   0.01  -0.01     0.00   0.00  -0.01    -0.03
0.00  -0.01
    34   1     0.00  -0.03   0.04     0.00  -0.05   0.06     0.09  -
0.09   0.08
    35   1     0.00   0.04   0.00     0.01   0.05  -0.01     0.08
0.23  -0.16
```

```
    36   1     0.01   0.04   0.00     0.01   0.05  -0.01     0.10  -
0.10   0.12
                     40                    41                    42
                      A                     A                     A
 Frequencies --   856.7861              870.6887
878.7758
 Red. masses --     1.6589                2.8612
1.4757
 Frc consts  --     0.7175                1.2780
0.6714
 IR Inten    --    10.5948                3.8425
2.0644
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.01  -0.05   0.00    -0.01   0.01   0.03     0.03
0.02   0.04
     2   6     0.08  -0.01  -0.03     0.02   0.21  -0.08     0.01
0.01  -0.01
     3   1     0.15  -0.09  -0.20    -0.01   0.18  -0.18     0.02
0.01  -0.01
     4   6     0.03   0.03  -0.03    -0.04  -0.09   0.01    -0.03  -
0.02  -0.04
     5   6     0.09  -0.04  -0.06     0.01  -0.01   0.03     0.00
0.00   0.00
     6   6    -0.01  -0.05  -0.03    -0.01   0.01   0.04    -0.01
0.00   0.00
     7   1     0.19   0.51   0.49    -0.07  -0.18  -0.13    -0.02  -
0.02  -0.02
     8   6     0.02   0.02   0.01    -0.02  -0.03  -0.03    -0.01
0.00   0.00
     9   1     0.07   0.05   0.22     0.04   0.01   0.11    -0.01
0.00  -0.02
    10   6    -0.03  -0.05   0.04    -0.01  -0.06  -0.03    -0.05  -
0.03  -0.06
    11   1    -0.03  -0.01   0.13     0.10   0.06   0.24     0.23
0.15   0.35
    12   6    -0.02   0.00   0.00     0.06   0.02  -0.08    -0.03  -
0.02  -0.03
    13   1    -0.01   0.03   0.03     0.16   0.03   0.05     0.14
0.11   0.23
    14   6    -0.03   0.03   0.02    -0.04   0.07   0.03     0.02
0.01   0.03
    15   1    -0.10  -0.03   0.00    -0.14   0.01  -0.14    -0.13  -
0.09  -0.19
    16   6    -0.03   0.07   0.00     0.03  -0.09   0.08     0.04
0.03   0.06
    17   1    -0.13   0.05  -0.06     0.00  -0.24  -0.21    -0.24  -
0.16  -0.34
    18   6     0.01  -0.03   0.02     0.01  -0.10  -0.01     0.00
0.01   0.05
    19   6     0.01   0.03   0.00     0.03   0.02   0.03     0.00  -
0.02  -0.04
```

```
    20   6    -0.02   0.04  -0.03    -0.03  -0.06  -0.04     0.00
0.03   0.07
    21   1    -0.04   0.10   0.08     0.07   0.12   0.35    -0.04  -
0.17  -0.35
    22   6    -0.03   0.01  -0.01    -0.07   0.04  -0.05    -0.01
0.02   0.03
    23   1    -0.04   0.02   0.08    -0.08   0.11   0.17    -0.04  -
0.11  -0.22
    24   6    -0.02   0.00   0.01     0.06   0.05   0.01     0.01  -
0.01  -0.04
    25   1    -0.05   0.02  -0.03     0.03  -0.05  -0.25     0.03
0.11   0.21
    26   6    -0.03  -0.05   0.04    -0.01  -0.07   0.11    -0.01  -
0.04  -0.06
    27   1    -0.10  -0.08  -0.04    -0.19  -0.24  -0.26     0.00
0.16   0.35
    28   6    -0.02   0.01   0.00     0.02  -0.02   0.02     0.00  -
0.01   0.00
    29   6     0.01   0.03   0.02    -0.02  -0.03   0.00     0.00  -
0.01   0.01
    30   8    -0.02  -0.02   0.01     0.02   0.06  -0.03     0.02
0.01  -0.01
    31   8    -0.01   0.00  -0.01     0.00  -0.01   0.01     0.00  -
0.01   0.00
    32   8     0.00   0.00   0.00     0.00  -0.01   0.00     0.00
0.00   0.00
    33   6     0.03  -0.02  -0.03     0.01   0.06  -0.01     0.00
0.00   0.00
    34   1    -0.07  -0.10   0.13    -0.01   0.15  -0.14     0.00
0.01  -0.01
    35   1    -0.07  -0.06   0.16     0.00  -0.04  -0.04    -0.01  -
0.01   0.01
    36   1    -0.07   0.29  -0.14    -0.03  -0.02  -0.05    -0.02
0.00  -0.01
                     43                     44                     45
                      A                      A                      A
 Frequencies --   886.1300               886.6091
905.8341
 Red. masses --     5.7394                 2.0490
7.8663
 Frc consts  --     2.6553                 0.9490
3.8029
 IR Inten    --    18.0113                 0.2099
125.8562
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.01   0.03  -0.01    -0.05  -0.03  -0.05     0.02  -
0.01  -0.03
     2   6     0.02   0.07  -0.02     0.02   0.12  -0.02     0.04  -
0.07  -0.01
     3   1     0.12   0.23   0.36     0.05   0.13  -0.01     0.05  -
0.10  -0.08
```

```
     4   6    -0.02  -0.02   0.05    0.03  -0.01   0.06    0.01
0.04   0.01
     5   6    -0.08   0.00   0.03    0.01  -0.04  -0.02   -0.05
0.01   0.01
     6   6     0.27  -0.01  -0.04   -0.02  -0.01   0.00    0.03
0.01  -0.05
     7   1     0.30   0.26   0.10    0.00   0.02   0.04   -0.09
0.36  -0.03
     8   6     0.31  -0.08   0.01   -0.04   0.01   0.00    0.20
0.02   0.00
     9   1     0.15  -0.23  -0.12    0.01   0.03   0.18    0.41
0.19   0.15
    10   6     0.00   0.02  -0.02    0.04  -0.02   0.07    0.00
0.05   0.00
    11   1     0.05   0.02  -0.01   -0.23  -0.15  -0.25   -0.04  -
0.01  -0.12
    12   6    -0.01   0.00   0.00    0.06   0.03  -0.01   -0.05  -
0.01   0.06
    13   1     0.02   0.04   0.05   -0.09  -0.10  -0.24   -0.14  -
0.02  -0.04
    14   6     0.03  -0.02  -0.02   -0.06   0.04  -0.02    0.04  -
0.05  -0.02
    15   1     0.08   0.03  -0.02    0.06   0.12   0.15    0.10  -
0.01   0.03
    16   6     0.03  -0.04   0.01   -0.04  -0.08  -0.02   -0.01
0.05  -0.05
    17   1     0.05  -0.07  -0.04    0.27   0.06   0.27    0.02
0.12   0.10
    18   6    -0.01  -0.03   0.02    0.02  -0.01   0.08   -0.02
0.01   0.00
    19   6     0.02  -0.03  -0.03    0.01  -0.03  -0.07    0.01  -
0.02  -0.01
    20   6    -0.02  -0.04   0.04    0.00   0.02   0.08   -0.01  -
0.01   0.02
    21   1     0.04  -0.09  -0.06   -0.02  -0.18  -0.33    0.02  -
0.03  -0.02
    22   6    -0.06   0.05   0.00   -0.03   0.04   0.02   -0.04
0.02   0.00
    23   1    -0.09  -0.03  -0.08   -0.06  -0.10  -0.24   -0.06  -
0.03  -0.04
    24   6     0.08   0.03  -0.02    0.02   0.01  -0.04    0.04
0.01  -0.01
    25   1     0.09   0.01   0.00    0.03   0.15   0.19    0.06  -
0.03   0.01
    26   6     0.01  -0.06   0.01   -0.02  -0.09  -0.04    0.01  -
0.01  -0.01
    27   1    -0.06  -0.01   0.10   -0.08   0.12   0.37    0.02
0.02   0.04
    28   6    -0.05   0.03   0.03    0.01  -0.01   0.00   -0.01  -
0.15   0.13
    29   6     0.03   0.11  -0.03   -0.01   0.00   0.01   -0.07  -
0.12   0.09
```

```
    30   8    -0.32  -0.11   0.07     0.03   0.01  -0.01    -0.08
0.46  -0.27
    31   8    -0.05   0.07  -0.06     0.01  -0.01   0.00    -0.02  -
0.10   0.07
    32   8    -0.04  -0.01   0.00     0.00   0.00   0.00    -0.03  -
0.19   0.08
    33   6    -0.03   0.04  -0.01     0.00   0.03  -0.03    -0.02  -
0.01   0.02
    34   1     0.06   0.05  -0.07    -0.01   0.00   0.02     0.06  -
0.01  -0.01
    35   1     0.05   0.15  -0.15    -0.01   0.04   0.00     0.03
0.04  -0.07
    36   1     0.06  -0.13   0.08     0.00   0.11  -0.05     0.03  -
0.11   0.07
                     46                     47                     48
                      A                      A                      A
 Frequencies --   910.2042               942.8967
963.7506
 Red. masses --     4.0057                 1.3352
1.3591
 Frc consts  --     1.9553                 0.6994
0.7437
 IR Inten    --     5.0887                13.6753
1.6960
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.04   0.01   0.06    -0.02   0.02   0.02    -0.01
0.00   0.00
     2   6    -0.18   0.02   0.05    -0.05   0.00  -0.01     0.00
0.00   0.00
     3   1    -0.39  -0.05  -0.13     0.14   0.26   0.60     0.03
0.03   0.07
     4   6     0.02  -0.05  -0.03    -0.01  -0.02   0.01     0.00
0.00   0.00
     5   6     0.13  -0.01  -0.03     0.02  -0.01   0.00     0.01
0.00   0.00
     6   6     0.10   0.01   0.03    -0.06   0.01  -0.06    -0.02
0.00  -0.01
     7   1     0.06  -0.11  -0.10    -0.06   0.37   0.12    -0.02
0.06   0.01
     8   6     0.09  -0.02  -0.03     0.02  -0.01   0.03     0.00
0.00   0.01
     9   1     0.20   0.04   0.31    -0.16  -0.13  -0.45    -0.04  -
0.03  -0.14
    10   6     0.02  -0.08   0.00     0.01  -0.02   0.01     0.01
0.00   0.02
    11   1    -0.03  -0.03   0.09    -0.04  -0.05  -0.06    -0.06  -
0.04  -0.10
    12   6     0.13   0.02  -0.10     0.02   0.00  -0.04    -0.01
0.00  -0.02
    13   1     0.19  -0.06  -0.06     0.11   0.05   0.08     0.06
0.04   0.07
```

```
    14    6    -0.11    0.10    0.03    -0.03    0.01   -0.01    -0.01   -
0.01   -0.01
    15    1    -0.18    0.01    0.06     0.03    0.04    0.08     0.05
0.03    0.08
    16    6    -0.02   -0.07    0.06     0.01   -0.03    0.03     0.01
0.00    0.02
    17    1     0.04   -0.12   -0.02    -0.02   -0.09   -0.08    -0.06   -
0.05   -0.09
    18    6     0.04    0.05   -0.02     0.01   -0.01    0.00     0.00
0.01    0.02
    19    6    -0.08    0.00   -0.03    -0.01    0.00    0.00     0.00
0.01    0.02
    20    6     0.05    0.08   -0.03     0.01    0.01    0.01     0.00   -
0.04   -0.09
    21    1    -0.05    0.06   -0.06    -0.02   -0.04   -0.08     0.06
0.23    0.48
    22    6     0.17   -0.09    0.04     0.02   -0.02   -0.02     0.01
0.03    0.06
    23    1     0.22   -0.05   -0.09     0.05    0.08    0.13    -0.03   -
0.18   -0.36
    24    6    -0.15   -0.05    0.04    -0.02   -0.01   -0.01     0.00
0.03    0.06
    25    1    -0.19    0.02    0.00    -0.02    0.05    0.07    -0.03   -
0.18   -0.36
    26    6    -0.02    0.11   -0.07     0.00    0.02    0.02    -0.01   -
0.04   -0.08
    27    1     0.13    0.13    0.00    -0.01   -0.04   -0.12     0.04
0.23    0.47
    28    6     0.02   -0.02    0.05    -0.04    0.01    0.00    -0.01
0.00    0.00
    29    6    -0.03    0.00    0.00     0.03   -0.01    0.01     0.01
0.00    0.00
    30    8    -0.10    0.04   -0.02     0.04    0.02   -0.02     0.01
0.00    0.00
    31    8    -0.02    0.02   -0.01     0.01   -0.02    0.02     0.00
0.00    0.00
    32    8    -0.02   -0.02    0.00     0.01   -0.02    0.01     0.00
0.00    0.00
    33    6     0.05   -0.02    0.00     0.01    0.01   -0.02     0.00
0.00   -0.01
    34    1    -0.09    0.00    0.02    -0.01    0.00    0.01     0.00   -
0.02    0.03
    35    1    -0.07   -0.20    0.19    -0.01    0.00    0.02    -0.01
0.02    0.02
    36    1    -0.09    0.19   -0.15    -0.01    0.07   -0.04     0.00
0.03   -0.01
                     49                     50                     51
                      A                      A                      A
 Frequencies --    968.5997               996.6542
1001.6958
 Red. masses --      1.3565                 1.2983
1.3024
```

This journal is © The Royal Society of Chemistry 2014

```
 Frc consts  --     0.7498                  0.7598
0.7699
 IR Inten    --     2.1238                  0.0319
0.0209
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.00   0.01   0.02     0.00   0.00   0.00     0.00
0.00   0.00
     2   6    -0.01   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     3   1     0.01   0.04   0.10     0.00   0.00   0.00     0.01
0.00   0.00
     4   6     0.01   0.01   0.02     0.00   0.00   0.00     0.00
0.00  -0.01
     5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     6   6    -0.02   0.00  -0.02     0.00   0.00   0.00     0.00
0.00   0.00
     7   1    -0.02   0.09   0.02     0.00  -0.01   0.00     0.00  -
0.01  -0.01
     8   6     0.01   0.00   0.01     0.00   0.00   0.00     0.00
0.00   0.00
     9   1    -0.06  -0.05  -0.20     0.01   0.01   0.03     0.01
0.01   0.03
    10   6    -0.05  -0.03  -0.07     0.00   0.00   0.00     0.03
0.02   0.05
    11   1     0.26   0.18   0.42     0.00   0.00   0.00    -0.19  -
0.13  -0.29
    12   6     0.05   0.03   0.04     0.00   0.00   0.00    -0.06  -
0.04  -0.08
    13   1    -0.19  -0.14  -0.30     0.00   0.00   0.00     0.31
0.22   0.46
    14   6     0.04   0.03   0.06     0.00   0.00   0.00     0.05
0.04   0.08
    15   1    -0.23  -0.16  -0.33     0.00   0.00   0.00    -0.31  -
0.21  -0.46
    16   6    -0.05  -0.04  -0.07     0.00   0.00   0.00    -0.03  -
0.02  -0.04
    17   1     0.27   0.18   0.40     0.00   0.00   0.00     0.18
0.13   0.27
    18   6     0.01   0.00   0.01     0.00   0.00   0.00     0.00
0.00   0.00
    19   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    20   6     0.00   0.00  -0.02     0.00   0.02   0.05     0.00
0.00   0.00
    21   1     0.01   0.04   0.08    -0.04  -0.16  -0.32     0.00
0.00   0.00
    22   6     0.01   0.00   0.01    -0.01  -0.04  -0.09     0.00
0.00   0.00
    23   1     0.00  -0.02  -0.05     0.05   0.26   0.52     0.00
0.00   0.00
```

```
    24   6     0.00   0.00   0.01     0.01   0.05   0.09     0.00
0.00   0.00
    25   1    -0.01  -0.04  -0.07    -0.04  -0.26  -0.54     0.00
0.00   0.00
    26   6     0.00   0.00  -0.02     0.00  -0.03  -0.05     0.00
0.00   0.00
    27   1     0.01   0.04   0.08     0.02   0.16   0.33     0.00
0.00   0.00
    28   6    -0.01   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    29   6     0.01   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    30   8     0.01   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    31   8     0.00  -0.01   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    32   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    33   6     0.00   0.00  -0.01     0.00   0.00   0.00     0.00
0.00   0.00
    34   1     0.00  -0.03   0.03     0.00  -0.01   0.01     0.00  -
0.01   0.01
    35   1     0.00   0.03   0.00     0.00   0.01   0.00     0.00
0.01   0.00
    36   1     0.02   0.04   0.00     0.00   0.00   0.00     0.01
0.00   0.01
                     52                     53                     54
                      A                      A                      A
 Frequencies --  1024.6874              1045.6288
1051.1525
 Red. masses --     1.4497                 1.5640
2.3571
 Frc consts  --     0.8968                 1.0075
1.5345
 IR Inten    --     4.4102                10.0977
5.4630
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.03  -0.01   0.01     0.02  -0.01   0.00     0.01
0.02  -0.02
     2   6    -0.02  -0.04  -0.07    -0.02  -0.02  -0.06    -0.02
0.01   0.01
     3   1     0.20   0.18   0.46     0.16   0.15   0.35    -0.11
0.02   0.03
     4   6    -0.01  -0.01   0.02     0.01   0.01  -0.03     0.05  -
0.02  -0.03
     5   6    -0.01  -0.04   0.01     0.03   0.11   0.04     0.02
0.01   0.00
     6   6     0.06   0.05  -0.03     0.00   0.01   0.03    -0.01
0.00   0.00
     7   1    -0.05   0.17  -0.12     0.03  -0.23  -0.05    -0.01
0.00   0.00
```

```
     8   6    -0.06  -0.03  -0.03    -0.01   0.01  -0.04     0.00
0.00   0.00
     9   1    -0.12  -0.15   0.72     0.16   0.15   0.20     0.00
0.00  -0.04
    10   6     0.00   0.01  -0.02    -0.01  -0.03   0.02     0.02  -
0.08   0.02
    11   1     0.05   0.03   0.03    -0.03  -0.01   0.07     0.22  -
0.15  -0.08
    12   6    -0.02  -0.01   0.02     0.00   0.01   0.00    -0.05  -
0.06   0.07
    13   1    -0.03  -0.03   0.01    -0.03   0.06  -0.03    -0.02  -
0.18   0.08
    14   6     0.01  -0.01   0.00     0.00   0.01   0.00    -0.07
0.12  -0.01
    15   1     0.00  -0.02  -0.02     0.02   0.04  -0.02    -0.02
0.20  -0.08
    16   6     0.00   0.03  -0.02     0.00  -0.02   0.02     0.03
0.03  -0.03
    17   1     0.03   0.04   0.00    -0.05  -0.02   0.01     0.20  -
0.03  -0.14
    18   6     0.03  -0.02   0.01    -0.02   0.02  -0.02     0.06
0.00   0.00
    19   6     0.00   0.01   0.02    -0.02   0.01   0.01     0.02  -
0.03   0.01
    20   6     0.00   0.01  -0.02     0.00  -0.05   0.02     0.05
0.08  -0.04
    21   1     0.00   0.05   0.05     0.03  -0.05   0.04     0.36
0.05  -0.06
    22   6     0.01  -0.01   0.01     0.00   0.01   0.00    -0.07
0.11  -0.05
    23   1     0.01  -0.01  -0.01     0.03   0.05  -0.03     0.01
0.24  -0.12
    24   6    -0.02  -0.01   0.01     0.02   0.02  -0.01    -0.12  -
0.11   0.06
    25   1    -0.01  -0.03   0.00     0.00   0.07  -0.03    -0.06  -
0.24   0.13
    26   6     0.00   0.01  -0.01     0.00  -0.02   0.02     0.04  -
0.06   0.03
    27   1    -0.02   0.03   0.02     0.02  -0.03   0.00     0.33  -
0.10   0.02
    28   6     0.03  -0.01   0.01     0.02   0.00   0.01     0.00
0.00   0.00
    29   6    -0.07  -0.01   0.02     0.00   0.00   0.00     0.00
0.00   0.00
    30   8     0.02  -0.01   0.00    -0.01   0.00   0.00     0.00
0.00   0.00
    31   8     0.01   0.01  -0.01     0.00   0.00   0.00     0.00
0.00   0.00
    32   8     0.00   0.00   0.00     0.00   0.01   0.00     0.00
0.00   0.00
    33   6     0.00   0.04   0.01    -0.03  -0.10  -0.08    -0.08
0.01   0.01
```

```
    34   1     0.00   0.15  -0.15     0.04  -0.46   0.45     0.15  -
0.05   0.01
    35   1     0.01  -0.06  -0.04    -0.02   0.31   0.04     0.07
0.24  -0.21
    36   1    -0.03  -0.07  -0.01     0.12   0.26   0.05     0.11  -
0.22   0.20
                     55                    56                    57
                      A                     A                     A
 Frequencies --  1055.9788             1070.0164
1078.7293
 Red. masses --     2.3933                1.7580
2.2193
 Frc consts  --     1.5724                1.1859
1.5216
 IR Inten    --     2.2376                4.8297
8.0432
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.04  -0.01   0.02    -0.01   0.01  -0.01    -0.01  -
0.01   0.00
     2   6     0.01   0.01   0.02     0.01  -0.01   0.05     0.02
0.04   0.03
     3   1    -0.04  -0.06  -0.15    -0.11  -0.12  -0.22    -0.09  -
0.06  -0.23
     4   6    -0.05   0.01   0.02     0.04   0.04  -0.04    -0.07  -
0.06   0.06
     5   6     0.01   0.01   0.03     0.01   0.09  -0.04     0.02  -
0.06   0.13
     6   6     0.01   0.02  -0.01     0.01   0.07  -0.01    -0.04
0.02   0.01
     7   1    -0.12   0.16  -0.12    -0.40   0.43  -0.36    -0.33
0.17  -0.27
     8   6     0.00  -0.03   0.01     0.05  -0.08   0.05     0.05  -
0.04   0.02
     9   1    -0.14  -0.17   0.11    -0.31  -0.42   0.22     0.02  -
0.09   0.12
    10   6    -0.03   0.10  -0.01     0.00  -0.06   0.03     0.03
0.06  -0.04
    11   1    -0.31   0.17   0.09     0.03  -0.08   0.00     0.15
0.01  -0.13
    12   6     0.08   0.08  -0.10     0.00   0.01   0.00    -0.04  -
0.04   0.04
    13   1     0.03   0.25  -0.12    -0.02   0.03  -0.01     0.02  -
0.18   0.08
    14   6     0.08  -0.15   0.01    -0.03   0.04   0.00     0.02
0.00  -0.01
    15   1     0.01  -0.28   0.14     0.00   0.09  -0.03     0.02
0.01  -0.02
    16   6    -0.04  -0.04   0.06     0.01  -0.03   0.01     0.02
0.05  -0.03
    17   1    -0.29   0.01   0.17     0.01  -0.03   0.00     0.15  -
0.01  -0.14
```

```
    18   6     0.04  -0.01  -0.01    -0.05   0.06  -0.03     0.06  -
0.08   0.02
    19   6     0.03  -0.01   0.00     0.00   0.01  -0.01     0.00  -
0.02  -0.01
    20   6     0.05   0.06  -0.03    -0.01  -0.06   0.03    -0.02
0.07  -0.02
    21   1     0.29   0.03  -0.07    -0.04  -0.07   0.01    -0.17
0.07  -0.04
    22   6    -0.07   0.09  -0.04     0.00   0.01   0.00     0.03  -
0.05   0.02
    23   1    -0.01   0.19  -0.08     0.02   0.03  -0.01    -0.05  -
0.16   0.09
    24   6    -0.09  -0.08   0.05     0.04   0.03  -0.02    -0.02
0.01   0.00
    25   1    -0.02  -0.22   0.11     0.02   0.08  -0.04    -0.02
0.03   0.00
    26   6     0.04  -0.05   0.03    -0.01  -0.03   0.02    -0.01
0.06  -0.02
    27   1     0.25  -0.08   0.01     0.01  -0.03   0.01    -0.18
0.06  -0.05
    28   6     0.00   0.00  -0.01    -0.05   0.02  -0.03    -0.06
0.03  -0.02
    29   6    -0.01  -0.01   0.00     0.00  -0.01  -0.02     0.05
0.01  -0.03
    30   8     0.01   0.00   0.00     0.04  -0.01   0.01     0.02
0.00   0.00
    31   8     0.00   0.01   0.00     0.00   0.02  -0.01    -0.01
0.00   0.00
    32   8     0.00   0.00   0.00     0.00  -0.02   0.01     0.00  -
0.01   0.00
    33   6     0.00  -0.01  -0.04     0.00  -0.06   0.04    -0.03
0.03  -0.12
    34   1     0.00  -0.10   0.11     0.00  -0.08   0.06     0.03  -
0.22   0.24
    35   1    -0.02   0.09   0.03    -0.01  -0.07   0.07     0.01
0.36  -0.08
    36   1     0.03   0.13  -0.03     0.01  -0.07   0.05     0.08
0.33  -0.05
                     58                     59                     60
                      A                      A                      A
 Frequencies --  1087.0973              1101.6851
1133.9204
 Red. masses --     1.9744                 1.6814
2.0498
 Frc consts  --     1.3747                 1.2024
1.5528
 IR Inten    --    28.1313                 0.0794
0.4236
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.01  -0.01   0.00    -0.01   0.00   0.00     0.04
0.05  -0.05
```

This journal is © The Royal Society of Chemistry 2014

```
     2   6    -0.01  -0.02  -0.03     0.00   0.00   0.00     0.06  -
0.01  -0.02
     3   1     0.07   0.07   0.18    -0.07   0.02   0.03    -0.09
0.03   0.04
     4   6     0.02   0.01   0.00    -0.08  -0.02   0.08    -0.02
0.08  -0.03
     5   6    -0.02  -0.02  -0.05    -0.06   0.01   0.01    -0.04
0.01   0.01
     6   6    -0.13  -0.03   0.06     0.01   0.00   0.00     0.00
0.00   0.00
     7   1    -0.36   0.02  -0.20     0.02  -0.03   0.00    -0.01  -
0.01  -0.01
     8   6     0.08  -0.05  -0.03     0.00   0.00   0.00     0.00
0.00   0.00
     9   1     0.59   0.38   0.29     0.00   0.00   0.01     0.02
0.02   0.04
    10   6    -0.01   0.00   0.00     0.03   0.00  -0.03     0.01  -
0.11   0.04
    11   1    -0.05   0.03   0.05     0.21  -0.04  -0.10     0.11  -
0.15  -0.01
    12   6     0.01   0.01  -0.01    -0.04  -0.03   0.04    -0.02
0.05  -0.01
    13   1    -0.01   0.03  -0.02    -0.01  -0.09   0.05    -0.18
0.42  -0.09
    14   6     0.00  -0.01   0.00     0.01   0.02  -0.02     0.02
0.02  -0.03
    15   1    -0.01  -0.03   0.02     0.08   0.11  -0.11     0.17
0.23  -0.22
    16   6    -0.01   0.00   0.00     0.03   0.00  -0.02    -0.02  -
0.09   0.06
    17   1    -0.05   0.02   0.04     0.20  -0.05  -0.10    -0.15  -
0.06   0.14
    18   6    -0.01   0.02   0.01    -0.09   0.05  -0.03    -0.03  -
0.07   0.04
    19   6    -0.01   0.00   0.00    -0.01   0.00   0.00     0.03  -
0.07   0.03
    20   6     0.01  -0.01   0.00     0.04  -0.02   0.01     0.03
0.10  -0.05
    21   1     0.07  -0.02   0.00     0.24  -0.04  -0.02     0.17
0.09  -0.06
    22   6    -0.01   0.02  -0.01    -0.04   0.04  -0.02    -0.03  -
0.04   0.02
    23   1     0.02   0.05  -0.03    -0.01   0.09  -0.04    -0.27  -
0.35   0.21
    24   6    -0.01  -0.01   0.00     0.01  -0.03   0.01     0.02  -
0.03   0.01
    25   1     0.00  -0.03   0.01     0.08  -0.16   0.06     0.17  -
0.31   0.13
    26   6     0.01  -0.01   0.00     0.03  -0.01   0.00    -0.02
0.10  -0.05
    27   1     0.06   0.00   0.03     0.22  -0.02   0.00    -0.17
0.12  -0.06
```

```
    28   6    -0.13   0.08   0.00     0.01   0.00   0.00     0.00
0.00   0.00
    29   6     0.13   0.04  -0.05     0.00   0.00   0.00     0.00
0.00   0.00
    30   8     0.01  -0.02   0.01     0.00   0.00   0.00     0.00
0.00   0.00
    31   8    -0.01  -0.02   0.02     0.00   0.00   0.00     0.00
0.00   0.00
    32   8     0.02  -0.01   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    33   6     0.02   0.02   0.04     0.12  -0.02  -0.03     0.01
0.00   0.00
    34   1    -0.04   0.15  -0.15    -0.24   0.01   0.06    -0.03
0.00   0.01
    35   1     0.00  -0.16   0.03    -0.13  -0.32   0.38     0.00  -
0.01   0.02
    36   1    -0.05  -0.11  -0.01    -0.17   0.41  -0.33    -0.01
0.01  -0.01
                      61                     62                     63
                       A                      A                      A
 Frequencies --  1180.2191              1192.1628
1202.9042
 Red. masses --     1.3795                 1.1648
1.1230
 Frc consts  --     1.1321                 0.9754
0.9574
 IR Inten    --     5.3539                 3.3447
0.4971
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.01  -0.02   0.02    -0.02   0.02   0.01     0.01  -
0.01   0.00
     2   6     0.00   0.04  -0.02     0.02  -0.01   0.00     0.00
0.00   0.00
     3   1     0.06   0.06   0.03     0.15  -0.04  -0.05    -0.02
0.00   0.00
     4   6     0.05  -0.02  -0.02    -0.01  -0.01   0.02    -0.02
0.02   0.00
     5   6     0.01   0.05  -0.03     0.03  -0.02   0.00    -0.01  -
0.03   0.01
     6   6     0.00   0.00   0.01     0.00   0.00   0.00     0.00
0.00   0.00
     7   1    -0.02   0.00  -0.02     0.01   0.00   0.01    -0.01
0.01  -0.01
     8   6     0.01   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     9   1    -0.04  -0.04  -0.02     0.01   0.01   0.02    -0.02  -
0.01  -0.01
    10   6    -0.04   0.04   0.01     0.02  -0.01  -0.02     0.00
0.00   0.01
    11   1    -0.33   0.14   0.16     0.30  -0.09  -0.15    -0.17
0.05   0.09
```

This journal is © The Royal Society of Chemistry 2014

12	6	0.02	-0.03	0.00	-0.02	0.04	0.00	0.01	-0.02	0.00
13	1	0.18	-0.39	0.07	-0.16	0.36	-0.07	0.13	-0.31	0.06
14	6	-0.02	0.00	0.02	-0.02	-0.02	0.02	0.03	0.02	-0.03
15	1	-0.13	-0.15	0.16	-0.15	-0.20	0.20	0.27	0.35	-0.35
16	6	0.03	0.03	-0.04	0.01	0.00	-0.01	-0.03	-0.01	0.03
17	1	0.13	0.01	-0.09	0.15	-0.04	-0.07	-0.31	0.08	0.17
18	6	-0.06	0.01	0.00	0.00	0.02	-0.01	0.02	0.00	0.00
19	6	-0.01	-0.03	0.01	-0.04	-0.01	0.00	0.00	0.00	0.00
20	6	0.05	0.02	-0.01	0.02	-0.01	0.01	0.00	0.00	0.00
21	1	0.47	-0.03	-0.04	0.30	-0.05	-0.02	0.12	-0.02	-0.01
22	6	-0.03	-0.03	0.02	-0.02	-0.03	0.01	-0.01	-0.01	0.01
23	1	-0.28	-0.36	0.21	-0.20	-0.26	0.15	-0.14	-0.17	0.10
24	6	0.02	-0.01	0.00	-0.03	0.03	-0.02	-0.03	0.03	-0.01
25	1	0.08	-0.11	0.05	-0.22	0.39	-0.18	-0.22	0.38	-0.17
26	6	-0.03	0.04	-0.02	0.03	-0.01	0.01	0.03	-0.02	0.01
27	1	-0.10	0.05	-0.02	0.29	-0.04	-0.01	0.30	-0.05	0.00
28	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
31	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
33	6	0.00	-0.02	0.01	-0.01	0.01	0.00	0.00	0.01	-0.01
34	1	0.01	-0.04	0.03	0.03	0.01	-0.02	-0.01	0.02	-0.02
35	1	0.00	-0.02	0.01	0.00	0.02	-0.03	-0.01	0.00	0.01
36	1	0.01	-0.04	0.03	0.01	-0.03	0.02	0.00	0.01	-0.01

	64	65	66
	A	A	A

This journal is © The Royal Society of Chemistry 2014

```
 Frequencies --  1222.9081              1255.3695
1263.1043
 Red. masses --     1.3627                 6.3697
1.7875
 Frc consts  --     1.2007                 5.9144
1.6802
 IR Inten    --     2.2271               254.6082
19.5809
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.09   0.02   0.06    -0.11   0.05   0.05     0.01
0.06  -0.03
     2   6     0.00   0.00   0.00    -0.04  -0.10   0.03     0.07
0.01  -0.03
     3   1     0.73  -0.16  -0.23    -0.03  -0.13   0.01     0.20  -
0.01  -0.06
     4   6    -0.01   0.03  -0.01    -0.05   0.05   0.01    -0.02
0.09  -0.02
     5   6     0.02  -0.01  -0.01    -0.01   0.03  -0.02    -0.02
0.00   0.00
     6   6     0.00   0.00   0.00    -0.14   0.07  -0.05    -0.02
0.00   0.00
     7   1    -0.01   0.01  -0.01    -0.20   0.19  -0.07    -0.06
0.04  -0.03
     8   6     0.00   0.00   0.00    -0.16  -0.08   0.01    -0.02
0.00   0.01
     9   1     0.00   0.00   0.00    -0.07   0.00   0.17    -0.04  -
0.02   0.02
    10   6     0.02   0.01  -0.02     0.00   0.01  -0.01    -0.02  -
0.02   0.02
    11   1     0.22  -0.04  -0.12     0.16  -0.03  -0.08    -0.35
0.08   0.19
    12   6     0.02   0.01  -0.02     0.02   0.00  -0.02     0.00  -
0.01   0.00
    13   1     0.09  -0.15   0.01     0.11  -0.18   0.02     0.05  -
0.11   0.02
    14   6     0.00   0.00   0.00     0.00   0.00   0.00    -0.02  -
0.01   0.02
    15   1     0.11   0.15  -0.14     0.04   0.06  -0.05    -0.05  -
0.06   0.07
    16   6     0.00  -0.02   0.01     0.02  -0.04   0.00     0.04  -
0.04  -0.01
    17   1    -0.13   0.02   0.08     0.14  -0.07  -0.05     0.36  -
0.14  -0.18
    18   6    -0.02  -0.03   0.01     0.11   0.05  -0.03    -0.07  -
0.09   0.05
    19   6    -0.11   0.01   0.00     0.16   0.05  -0.03    -0.05  -
0.08   0.04
    20   6     0.02  -0.02   0.01     0.01   0.00   0.00    -0.03
0.03  -0.01
    21   1     0.23  -0.05  -0.01     0.03   0.01   0.00    -0.37
0.07   0.01
```

```
    22   6     0.02  -0.02   0.01    -0.04   0.01   0.00     0.02
0.00   0.00
    23   1     0.14   0.13  -0.08    -0.23  -0.22   0.14     0.13
0.14  -0.08
    24   6     0.00   0.00   0.00     0.00  -0.01   0.01    -0.02
0.02  -0.01
    25   1     0.10  -0.19   0.08    -0.06   0.10  -0.04    -0.03
0.05  -0.02
    26   6     0.01   0.02  -0.01    -0.05  -0.04   0.02     0.07
0.04  -0.02
    27   1    -0.13   0.03  -0.01    -0.38  -0.01   0.05     0.56  -
0.01  -0.05
    28   6     0.00   0.00   0.00     0.34  -0.14   0.07     0.05  -
0.02   0.01
    29   6     0.00   0.00   0.00     0.33   0.09  -0.07     0.05
0.01  -0.01
    30   8     0.00   0.00   0.00    -0.21   0.03  -0.01    -0.03
0.00   0.00
    31   8     0.00   0.00   0.00    -0.03  -0.06   0.05    -0.01  -
0.01   0.01
    32   8     0.00   0.00   0.00    -0.03   0.06  -0.03    -0.01
0.01   0.00
    33   6    -0.01   0.00   0.00     0.00  -0.01   0.01     0.00
0.00   0.00
    34   1     0.03   0.00  -0.01     0.00   0.00   0.00    -0.01
0.00   0.00
    35   1     0.02   0.03  -0.05     0.01  -0.02   0.00    -0.02  -
0.02   0.03
    36   1     0.02  -0.05   0.04    -0.01  -0.02   0.01    -0.01
0.00  -0.01
                     67                     68                     69
                      A                      A                      A
 Frequencies --  1269.0449              1314.6891
1332.5936
 Red. masses --     3.0885                 1.6654
5.2902
 Frc consts  --     2.9306                 1.6960
5.5350
 IR Inten    --    31.8932                 0.4456
21.4283
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.14   0.14   0.05    -0.09   0.01   0.06    -0.03  -
0.21   0.10
     2   6     0.01  -0.14   0.02    -0.01  -0.01  -0.01     0.00
0.14  -0.01
     3   1     0.11  -0.18   0.00     0.01   0.00   0.05     0.09
0.14  -0.02
     4   6    -0.10   0.13   0.00     0.09  -0.06  -0.03    -0.09  -
0.02   0.09
     5   6    -0.01   0.03  -0.01     0.01  -0.02   0.03    -0.05
0.31  -0.24
```

This journal is © The Royal Society of Chemistry 2014

```
     6   6     0.03   0.00  -0.02    -0.01   0.01   0.00    -0.02
0.03  -0.04
     7   1     0.20  -0.12   0.12     0.03  -0.07   0.02     0.14  -
0.06   0.11
     8   6     0.02  -0.02  -0.03     0.01   0.00  -0.01     0.01  -
0.04   0.01
     9   1     0.24   0.16   0.08    -0.02  -0.03   0.06     0.08
0.02  -0.01
    10   6    -0.02   0.00   0.01    -0.02   0.02   0.01     0.07
0.04  -0.06
    11   1    -0.01   0.01   0.01     0.37  -0.10  -0.20     0.32  -
0.03  -0.20
    12   6     0.05   0.00  -0.03     0.02   0.02  -0.02    -0.04
0.06   0.01
    13   1     0.18  -0.31   0.02     0.10  -0.16   0.01     0.02  -
0.10   0.03
    14   6    -0.01  -0.02   0.01    -0.01   0.03  -0.01     0.02  -
0.04   0.01
    15   1     0.03   0.03  -0.04    -0.10  -0.09   0.11     0.09
0.05  -0.09
    16   6     0.05  -0.08   0.00     0.02   0.01  -0.01     0.01
0.03  -0.03
    17   1     0.47  -0.21  -0.21    -0.38   0.13   0.19    -0.07
0.07   0.03
    18   6     0.08   0.01  -0.02    -0.11  -0.02   0.02     0.16  -
0.08   0.04
    19   6     0.16   0.02  -0.02     0.10  -0.03   0.00     0.02  -
0.21   0.09
    20   6     0.01   0.01  -0.01     0.04   0.01  -0.01    -0.08
0.07  -0.03
    21   1    -0.24   0.05   0.00    -0.43   0.06   0.02    -0.31
0.10  -0.01
    22   6    -0.05   0.02   0.00    -0.02   0.03  -0.01     0.06
0.04  -0.03
    23   1    -0.17  -0.14   0.09    -0.15  -0.13   0.08    -0.06  -
0.10   0.05
    24   6    -0.01   0.00   0.00     0.02   0.03  -0.01    -0.03  -
0.05   0.03
    25   1    -0.07   0.10  -0.04     0.11  -0.15   0.06    -0.15
0.17  -0.07
    26   6    -0.02  -0.04   0.02    -0.02   0.01   0.00    -0.01
0.04  -0.02
    27   1    -0.18  -0.02   0.03     0.44  -0.03  -0.02     0.06
0.04  -0.01
    28   6    -0.12   0.06  -0.01     0.00   0.00   0.00    -0.02
0.02   0.00
    29   6    -0.12  -0.03   0.04     0.00   0.00   0.00    -0.01
0.00   0.01
    30   8     0.07  -0.01   0.00     0.00   0.00   0.00     0.01
0.00   0.00
    31   8     0.02   0.01  -0.01     0.00   0.00   0.00     0.01  -
0.01   0.00
```

```
    32   8     0.02  -0.01   0.00     0.00   0.00   0.00     0.01
0.00   0.00
    33   6     0.00  -0.02   0.01     0.00   0.02  -0.02     0.02  -
0.08   0.06
    34   1     0.00  -0.01   0.00     0.00  -0.02   0.03    -0.05  -
0.10   0.13
    35   1     0.01   0.01  -0.01    -0.03   0.00   0.03    -0.06  -
0.23   0.17
    36   1    -0.02   0.02  -0.01     0.04  -0.02   0.02     0.01  -
0.25   0.08
                     70                    71                    72
                      A                     A                     A
 Frequencies --  1335.3764             1356.3911
1376.5987
 Red. masses --     1.7661                3.6685
6.9715
 Frc consts  --     1.8556                3.9766
7.7838
 IR Inten    --     5.3498               21.0537
0.2961
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.00  -0.01   0.00    -0.06   0.05   0.03     0.01
0.24  -0.12
     2   6    -0.01   0.01   0.00     0.15  -0.02  -0.04     0.09  -
0.02  -0.02
     3   1     0.02   0.00  -0.01    -0.48   0.12   0.15     0.50  -
0.10  -0.14
     4   6     0.01  -0.01  -0.01    -0.16  -0.05   0.14     0.06  -
0.18   0.05
     5   6    -0.01   0.01   0.01     0.30  -0.04  -0.10    -0.02  -
0.02   0.02
     6   6     0.16  -0.07   0.02     0.01   0.00  -0.01    -0.01  -
0.01   0.01
     7   1    -0.30   0.51  -0.28     0.00   0.06   0.02    -0.02  -
0.01   0.00
     8   6    -0.15  -0.06   0.05    -0.03  -0.01   0.01     0.01
0.01  -0.01
     9   1     0.39   0.48  -0.34     0.08   0.08   0.02    -0.04  -
0.03   0.03
    10   6     0.00   0.00   0.00     0.03   0.00  -0.02    -0.17
0.05   0.10
    11   1     0.03  -0.01  -0.02    -0.05   0.03   0.03     0.11  -
0.03  -0.07
    12   6     0.00   0.00   0.00     0.00   0.02  -0.01     0.09  -
0.13   0.00
    13   1     0.00  -0.01   0.00     0.03  -0.04   0.00     0.05  -
0.02  -0.02
    14   6     0.00   0.01   0.00     0.02  -0.05   0.01     0.09
0.10  -0.11
    15   1    -0.02  -0.02   0.02     0.20   0.20  -0.23    -0.09  -
0.15   0.14
```

```
    16   6     0.00   0.00   0.00    -0.03   0.02   0.00    -0.12
0.01   0.08
    17   1    -0.04   0.02   0.02     0.07   0.00  -0.03     0.01  -
0.04   0.01
    18   6     0.00   0.00   0.00    -0.14   0.12  -0.05     0.09
0.19  -0.11
    19   6     0.01  -0.01   0.00    -0.07  -0.07   0.03    -0.01  -
0.25   0.13
    20   6     0.00   0.00   0.00     0.02   0.00   0.00    -0.23
0.02   0.01
    21   1    -0.03   0.00   0.00    -0.11   0.01   0.00     0.15  -
0.02   0.01
    22   6     0.00   0.01   0.00     0.01  -0.01   0.00     0.14
0.11  -0.07
    23   1    -0.02  -0.02   0.01     0.02   0.00  -0.01     0.03  -
0.03   0.01
    24   6     0.00   0.00   0.00     0.02   0.03  -0.02     0.11  -
0.16   0.07
    25   1     0.00   0.00   0.00     0.17  -0.24   0.10    -0.08
0.20  -0.09
    26   6    -0.01   0.00   0.00    -0.04  -0.01   0.01    -0.18
0.04  -0.01
    27   1     0.05   0.00   0.00     0.05  -0.02  -0.01     0.06
0.03  -0.01
    28   6     0.02  -0.01   0.02     0.01   0.00   0.00     0.00
0.00   0.00
    29   6    -0.05  -0.03   0.01     0.00   0.00   0.00     0.01
0.00   0.00
    30   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    31   8    -0.01   0.03  -0.02     0.00   0.00   0.00     0.00
0.00   0.00
    32   8     0.01   0.03  -0.02     0.00   0.00   0.00     0.00
0.00   0.00
    33   6     0.00   0.00   0.00    -0.08   0.01   0.02     0.03
0.00  -0.01
    34   1     0.00  -0.01   0.00     0.31  -0.04  -0.05    -0.08
0.02   0.00
    35   1    -0.01  -0.01   0.02     0.04  -0.02  -0.21     0.00
0.01   0.05
    36   1     0.01   0.02   0.00     0.11  -0.13   0.20    -0.02
0.05  -0.06
                     73                     74                     75
                      A                      A                      A
 Frequencies --   1394.6828              1413.6731
1414.8134
 Red. masses --      6.4282                 2.1710
2.5552
 Frc consts  --      7.3670                 2.5563
3.0135
 IR Inten    --      4.5298                 4.2483
8.3290
```

This journal is © The Royal Society of Chemistry 2014

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.03	-0.14	0.07	-0.02	0.06	-0.02	0.05	0.01	-0.04
2	6	0.00	0.07	0.01	0.12	-0.02	-0.01	-0.09	0.03	0.05
3	1	-0.01	0.06	-0.02	-0.33	0.04	0.03	0.27	-0.10	-0.17
4	6	0.01	0.19	-0.11	0.01	-0.03	0.01	0.02	-0.06	0.01
5	6	0.00	-0.18	0.17	-0.03	0.02	0.02	0.03	0.01	0.00
6	6	-0.02	0.09	-0.07	-0.02	0.13	-0.09	-0.03	0.17	-0.12
7	1	0.19	-0.12	0.06	0.23	-0.11	0.08	0.30	-0.15	0.10
8	6	-0.02	-0.10	0.04	-0.03	-0.14	0.06	-0.03	-0.18	0.08
9	1	0.18	0.07	-0.02	0.24	0.09	0.00	0.28	0.09	-0.04
10	6	0.17	-0.09	-0.08	-0.04	-0.02	0.04	0.01	0.02	-0.02
11	1	-0.26	0.04	0.16	0.12	-0.07	-0.05	-0.23	0.10	0.11
12	6	-0.09	0.15	0.00	-0.01	0.04	-0.01	0.03	-0.09	0.02
13	1	-0.03	-0.04	0.03	0.11	-0.27	0.05	-0.15	0.33	-0.05
14	6	-0.12	-0.09	0.13	0.01	0.04	-0.02	0.01	0.01	-0.01
15	1	-0.02	0.07	-0.03	-0.14	-0.18	0.19	0.10	0.14	-0.14
16	6	0.18	-0.03	-0.10	0.05	-0.03	-0.02	-0.08	0.05	0.03
17	1	-0.21	0.09	0.10	-0.28	0.07	0.16	0.17	-0.03	-0.11
18	6	0.00	0.15	-0.09	-0.02	-0.03	0.02	-0.01	-0.03	0.02
19	6	0.02	-0.10	0.04	-0.05	0.01	0.00	0.02	0.05	-0.03
20	6	-0.17	-0.02	0.03	-0.03	0.03	-0.01	0.04	-0.03	0.01
21	1	0.26	-0.07	0.01	0.26	0.00	-0.03	-0.08	-0.03	0.02
22	6	0.11	0.10	-0.06	-0.03	-0.07	0.04	0.02	0.02	-0.01
23	1	-0.01	-0.07	0.03	0.22	0.26	-0.15	-0.12	-0.16	0.09
24	6	0.11	-0.12	0.05	0.00	-0.01	0.00	-0.01	0.04	-0.02
25	1	0.03	0.04	-0.03	-0.11	0.21	-0.09	0.12	-0.20	0.09

```
    26   6    -0.19   0.04   0.00     0.08   0.01  -0.01    -0.05
0.00   0.00
    27   1     0.28  -0.01  -0.02    -0.23   0.05  -0.01     0.28  -
0.04   0.00
    28   6    -0.02   0.01   0.00    -0.01   0.01   0.00    -0.02
0.02   0.01
    29   6    -0.02   0.00   0.01    -0.01   0.00   0.01    -0.02
0.00   0.02
    30   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    31   8     0.01  -0.01   0.01     0.01  -0.02   0.01     0.02  -
0.02   0.01
    32   8     0.01   0.01  -0.01     0.01   0.01  -0.01     0.02
0.02  -0.01
    33   6     0.00   0.03  -0.03     0.01   0.00  -0.01    -0.01
0.02  -0.01
    34   1     0.00   0.09  -0.12    -0.07  -0.02   0.06     0.08  -
0.08   0.09
    35   1     0.03   0.16  -0.06    -0.01   0.01   0.04    -0.05  -
0.12   0.02
    36   1    -0.01   0.18  -0.05     0.00  -0.07  -0.01     0.04  -
0.06   0.04
                     76                    77                    78
                      A                     A                     A
 Frequencies --  1437.5156             1488.3316
1493.7697
 Red. masses --     1.2698                1.8332
2.3732
 Frc consts  --     1.5461                2.3925
3.1199
 IR Inten    --    15.4249               12.6950
5.8763
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.01   0.00   0.00     0.03  -0.08   0.02     0.10  -
0.01  -0.06
     2   6     0.00  -0.01   0.00    -0.01   0.00   0.00     0.00
0.00   0.01
     3   1    -0.01   0.00   0.01    -0.16   0.03   0.05    -0.03  -
0.01  -0.02
     4   6     0.00   0.01  -0.01     0.00   0.06  -0.04    -0.09
0.06   0.03
     5   6    -0.01  -0.02   0.02     0.02   0.00  -0.01     0.00  -
0.01   0.00
     6   6     0.00  -0.02   0.01     0.00   0.00   0.00     0.00
0.00  -0.01
     7   1    -0.03   0.02  -0.01     0.00  -0.01   0.00     0.01
0.00   0.01
     8   6     0.00   0.02  -0.01     0.00   0.00   0.00     0.00
0.00   0.01
     9   1    -0.03   0.00   0.01     0.00  -0.01   0.00     0.00  -
0.01  -0.01
```

This journal is © The Royal Society of Chemistry 2014

```
    10   6     0.01   0.00   0.00    -0.08   0.04   0.04    -0.04  -
0.05   0.05
    11   1    -0.02   0.01   0.01     0.31  -0.09  -0.17     0.12  -
0.11  -0.04
    12   6     0.00   0.00   0.00     0.02   0.02  -0.02    -0.06
0.09   0.00
    13   1     0.00   0.01   0.00     0.10  -0.15   0.00     0.13  -
0.40   0.09
    14   6    -0.01   0.00   0.01     0.04  -0.02  -0.02     0.07
0.05  -0.07
    15   1     0.00   0.00   0.00     0.07   0.00  -0.04    -0.17  -
0.30   0.26
    16   6     0.01   0.00   0.00    -0.08   0.00   0.05     0.02  -
0.07   0.02
    17   1     0.01  -0.01  -0.01     0.26  -0.11  -0.14    -0.12  -
0.03   0.10
    18   6     0.01   0.00   0.00    -0.02  -0.07   0.04     0.11
0.00  -0.02
    19   6     0.01   0.01   0.00     0.06   0.06  -0.03    -0.10
0.05  -0.01
    20   6    -0.02   0.00   0.00    -0.10   0.01   0.00     0.01  -
0.06   0.03
    21   1     0.06   0.00   0.00     0.38  -0.03  -0.02    -0.06  -
0.07   0.04
    22   6     0.00   0.00   0.00     0.01  -0.04   0.02     0.09
0.05  -0.03
    23   1     0.03   0.03  -0.02     0.16   0.16  -0.09    -0.17  -
0.31   0.17
    24   6     0.01  -0.01   0.00     0.06  -0.01   0.00    -0.07
0.08  -0.03
    25   1    -0.01   0.03  -0.02     0.05   0.04  -0.02     0.18  -
0.39   0.18
    26   6    -0.01   0.00   0.00    -0.08   0.04  -0.01    -0.05  -
0.05   0.03
    27   1    -0.04   0.01   0.00     0.29   0.01  -0.02     0.21  -
0.09   0.03
    28   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    29   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    30   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    31   8     0.00   0.01   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    32   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    33   6     0.01   0.13  -0.06    -0.04   0.00   0.01     0.00
0.01  -0.01
    34   1     0.08  -0.32   0.52     0.40  -0.03  -0.12     0.03  -
0.01   0.01
    35   1    -0.16  -0.54   0.08    -0.03  -0.23  -0.08    -0.03  -
0.05   0.03
```

```
    36   1     0.05  -0.50   0.04     0.10   0.28   0.10     0.03  -
0.03   0.03
                     79                    80                    81
                      A                     A                     A
 Frequencies --  1511.2419             1522.7582
1543.4377
 Red. masses --     1.2098                1.5669
1.5994
 Frc consts  --     1.6279                2.1407
2.2449
 IR Inten    --     0.7684                8.5611
2.4691
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.02   0.02  -0.02     0.04  -0.06   0.00     0.00
0.03  -0.01
     2   6    -0.03   0.01   0.01     0.00   0.03  -0.01    -0.05  -
0.01   0.02
     3   1     0.15  -0.03  -0.04     0.01   0.04   0.00     0.10  -
0.05  -0.03
     4   6    -0.01  -0.01   0.02     0.03   0.04  -0.04    -0.06  -
0.02   0.05
     5   6    -0.02   0.00   0.00     0.01  -0.03   0.03     0.05
0.04  -0.03
     6   6     0.00   0.00   0.00     0.00   0.03  -0.01     0.00  -
0.02   0.01
     7   1     0.00  -0.01   0.00     0.03  -0.01  -0.01    -0.02
0.02   0.00
     8   6     0.00   0.00   0.00     0.00  -0.03   0.02     0.00
0.01  -0.01
     9   1     0.00   0.00   0.00     0.03   0.00  -0.03    -0.02
0.00   0.01
    10   6     0.03  -0.02  -0.01    -0.06   0.01   0.03     0.05  -
0.02  -0.03
    11   1    -0.10   0.02   0.06     0.21  -0.07  -0.11    -0.17
0.05   0.09
    12   6    -0.02   0.00   0.01     0.01   0.04  -0.02    -0.03  -
0.02   0.03
    13   1    -0.02  -0.01   0.02     0.08  -0.13   0.00    -0.06
0.03   0.03
    14   6     0.00   0.03  -0.02     0.02  -0.04   0.01     0.02
0.06  -0.04
    15   1    -0.07  -0.07   0.09     0.07   0.02  -0.06    -0.12  -
0.12   0.14
    16   6     0.03  -0.02  -0.01    -0.06   0.02   0.03     0.04  -
0.04  -0.01
    17   1    -0.15   0.03   0.08     0.20  -0.06  -0.10    -0.21
0.05   0.14
    18   6    -0.02   0.02  -0.01    -0.04   0.05  -0.02    -0.01  -
0.04   0.02
    19   6     0.00  -0.03   0.02    -0.04  -0.04   0.02     0.08
0.03  -0.02
```

```
    20   6     0.04   0.00  -0.01     0.06  -0.01   0.00    -0.04
0.02  -0.01
    21   1    -0.16   0.03   0.00    -0.22   0.01   0.01     0.17
0.00  -0.02
    22   6    -0.02   0.02  -0.01     0.00   0.04  -0.02    -0.02  -
0.04   0.02
    23   1    -0.05  -0.01   0.01    -0.10  -0.08   0.05     0.10
0.11  -0.06
    24   6    -0.01  -0.03   0.02    -0.02  -0.03   0.02     0.04
0.01  -0.01
    25   1    -0.08   0.10  -0.04    -0.08   0.06  -0.03     0.04
0.02  -0.01
    26   6     0.05   0.00  -0.01     0.06   0.00   0.00    -0.06
0.02   0.00
    27   1    -0.20   0.03   0.01    -0.19   0.03   0.01     0.22
0.00   0.00
    28   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    29   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    30   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    31   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    32   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    33   6    -0.04   0.00   0.01     0.01   0.02   0.04     0.00  -
0.01   0.06
    34   1     0.60  -0.06  -0.14    -0.01  -0.12   0.21    -0.01  -
0.10   0.17
    35   1    -0.04  -0.42  -0.11     0.25  -0.06  -0.50     0.26
0.00  -0.51
    36   1     0.13   0.44   0.12    -0.42  -0.01  -0.37    -0.42  -
0.01  -0.36
                     82                     83                     84
                      A                      A                      A
 Frequencies --  1547.4233              1595.6854
1608.8529
 Red. masses --     2.5555                 4.8715
6.5880
 Frc consts  --     3.6053                 7.3082
10.0470
 IR Inten    --     0.5438                 1.8970
2.1765
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.11   0.05   0.05     0.09   0.10  -0.11    -0.04  -
0.19   0.11
     2   6     0.14  -0.04  -0.03    -0.11   0.02   0.03     0.00
0.06  -0.03
     3   1    -0.29   0.05   0.08     0.33  -0.07  -0.10     0.03
0.08   0.03
```

```
     4   6     0.08  -0.05  -0.03     0.05  -0.14   0.03    -0.02
0.20  -0.09
     5   6    -0.13   0.05   0.03    -0.06   0.01   0.01    -0.01  -
0.08   0.04
     6   6     0.00  -0.01   0.00     0.00   0.00   0.00     0.00
0.03  -0.02
     7   1    -0.01   0.00   0.00     0.00   0.00   0.00     0.03  -
0.02  -0.01
     8   6     0.00   0.01  -0.01     0.00   0.00   0.00     0.00  -
0.03   0.03
     9   1     0.00   0.00   0.02     0.00   0.00   0.00     0.03
0.00  -0.04
    10   6     0.00   0.03  -0.02     0.00  -0.11   0.05    -0.01
0.11  -0.04
    11   1    -0.04   0.05   0.00     0.04  -0.13   0.04     0.02
0.11  -0.07
    12   6     0.06  -0.06  -0.01    -0.06   0.23  -0.06     0.05  -
0.21   0.06
    13   1    -0.06   0.22  -0.06     0.17  -0.34   0.03    -0.15
0.27  -0.02
    14   6    -0.07  -0.03   0.07    -0.04  -0.17   0.11     0.07
0.17  -0.13
    15   1     0.07   0.19  -0.14     0.18   0.11  -0.17    -0.17  -
0.16   0.19
    16   6     0.03   0.03  -0.04    -0.03   0.09  -0.03    -0.02  -
0.10   0.06
    17   1    -0.04   0.07   0.00     0.12   0.06  -0.11     0.00  -
0.12   0.05
    18   6     0.12  -0.02   0.00     0.08   0.10  -0.06     0.06
0.20  -0.11
    19   6    -0.08   0.02   0.00     0.08  -0.13   0.05     0.02  -
0.21   0.10
    20   6    -0.06  -0.02   0.01     0.01   0.10  -0.05     0.03
0.11  -0.05
    21   1     0.12  -0.04   0.01     0.07   0.11  -0.06     0.00
0.13  -0.06
    22   6     0.08   0.00  -0.01    -0.10  -0.19   0.10    -0.10  -
0.20   0.11
    23   1    -0.01  -0.14   0.07     0.23   0.25  -0.14     0.23
0.22  -0.13
    24   6    -0.07   0.10  -0.04    -0.01   0.17  -0.08    -0.05
0.21  -0.10
    25   1     0.13  -0.28   0.13     0.18  -0.16   0.06     0.19  -
0.23   0.10
    26   6    -0.01  -0.05   0.02    -0.05  -0.07   0.04     0.00  -
0.11   0.06
    27   1     0.16  -0.07   0.04     0.14  -0.10   0.04     0.01  -
0.12   0.06
    28   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00  -
0.01   0.00
    29   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.01   0.00
```

```
    30   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    31   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    32   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    33   6     0.00  -0.01   0.03     0.01   0.00   0.00     0.00
0.01  -0.01
    34   1     0.29  -0.10   0.05     0.03  -0.01   0.00    -0.01
0.01  -0.01
    35   1     0.11  -0.29  -0.30     0.00  -0.06   0.00    -0.03  -
0.01   0.05
    36   1    -0.20   0.29  -0.20    -0.02   0.07  -0.04     0.04  -
0.02   0.03
                     85                     86                     87
                      A                      A                      A
 Frequencies --  1654.2751              1659.0402
1811.3375
 Red. masses --     5.5532                 5.5255
12.5933
 Frc consts  --     8.9539                 8.9606
24.3438
 IR Inten    --     0.7807                 4.7161
582.0313
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6    -0.10   0.02   0.06    -0.16   0.03   0.10    -0.01
0.00   0.00
     2   6     0.10  -0.02  -0.03     0.03  -0.02  -0.01    -0.01  -
0.01  -0.01
     3   1    -0.19   0.04   0.05    -0.05   0.00   0.04     0.02
0.01   0.02
     4   6     0.08  -0.02  -0.04     0.14  -0.06  -0.07     0.00
0.00   0.00
     5   6    -0.06   0.01   0.01    -0.02   0.00   0.01     0.00
0.01   0.01
     6   6     0.00   0.00   0.00     0.00   0.00   0.01     0.05  -
0.06   0.03
     7   1     0.00   0.00   0.00     0.00  -0.01  -0.01    -0.06
0.12  -0.06
     8   6     0.00   0.00   0.00     0.00   0.00  -0.01    -0.03  -
0.04   0.03
     9   1     0.00   0.00   0.00     0.00   0.00   0.02     0.06
0.07  -0.06
    10   6     0.12  -0.05  -0.06     0.24  -0.11  -0.12     0.01
0.00   0.00
    11   1    -0.16   0.04   0.09    -0.32   0.07   0.19     0.00
0.01   0.01
    12   6    -0.07   0.05   0.03    -0.16   0.13   0.05     0.00
0.00   0.00
    13   1    -0.01  -0.11   0.06    -0.02  -0.25   0.12     0.00
0.00   0.00
```

```
    14    6     0.08   0.02  -0.07     0.17   0.04  -0.13     0.00
0.00   0.00
    15    1    -0.02  -0.13   0.08    -0.02  -0.26   0.15     0.00
0.00   0.00
    16    6    -0.12   0.02   0.07    -0.24   0.04   0.15     0.00
0.00   0.00
    17    1     0.16  -0.07  -0.08     0.31  -0.14  -0.15     0.00
0.00  -0.01
    18    6     0.18  -0.01  -0.01    -0.09   0.00   0.01    -0.01
0.00   0.00
    19    6    -0.21   0.05  -0.01     0.09  -0.02   0.00     0.01
0.00   0.00
    20    6     0.28  -0.01  -0.02    -0.16   0.00   0.02    -0.01
0.00   0.00
    21    1    -0.37   0.06   0.00     0.20  -0.04   0.00     0.01
0.00   0.00
    22    6    -0.18  -0.04   0.04     0.10   0.03  -0.02     0.00
0.00   0.00
    23    1     0.01   0.23  -0.11    -0.01  -0.14   0.06     0.00
0.00   0.00
    24    6     0.18  -0.11   0.04    -0.10   0.05  -0.02     0.00
0.00   0.00
    25    1     0.00   0.26  -0.13     0.00  -0.14   0.07     0.00
0.00   0.00
    26    6    -0.27   0.07  -0.01     0.15  -0.03   0.00     0.00
0.00   0.00
    27    1     0.37   0.01  -0.03    -0.20   0.00   0.01    -0.01
0.00   0.00
    28    6     0.00   0.00   0.00     0.00   0.00   0.00     0.25
0.36  -0.17
    29    6     0.00   0.00   0.00     0.00   0.00   0.00    -0.32
0.47  -0.33
    30    8     0.00   0.00   0.00     0.00   0.00   0.00     0.01
0.01   0.00
    31    8     0.00   0.00   0.00     0.00   0.00   0.00     0.17  -
0.32   0.22
    32    8     0.00   0.00   0.00     0.00   0.00   0.00    -0.14  -
0.25   0.12
    33    6     0.01   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    34    1     0.01  -0.01   0.01    -0.01   0.00  -0.01     0.03  -
0.03   0.03
    35    1     0.00  -0.05   0.00    -0.01   0.01   0.03     0.01  -
0.08  -0.03
    36    1    -0.02   0.04  -0.03     0.02   0.02   0.01    -0.01
0.00  -0.01
                     88                    89                    90
                      A                     A                     A
 Frequencies --  1872.2060             3035.6942
3116.7058
 Red. masses --    12.5196                1.0507
1.0842
```

This journal is © The Royal Society of Chemistry 2014

Frc consts	--	25.8552			5.7049					
6.2051										
IR Inten	--	380.6563			17.1756					
5.5731										
Atom	AN	X	Y	Z	X	Y	Z	X	Y	
Z										
1	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
2	6	0.00	0.00	-0.01	0.00	0.00	0.00	0.00		
0.00	0.00									
3	1	0.02	0.02	0.02	0.00	0.00	0.00	0.00		
0.00	0.00									
4	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
5	6	0.00	-0.01	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
6	6	-0.04	0.03	-0.02	0.00	0.00	0.00	0.00		
0.00	0.00									
7	1	0.05	-0.09	0.07	0.00	0.00	0.00	0.00		
0.00	0.00									
8	6	-0.05	-0.04	0.02	0.00	0.00	0.00	0.00		
0.00	0.00									
9	1	0.09	0.12	-0.04	0.00	0.00	0.00	0.00		
0.00	0.00									
10	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
11	1	0.00	0.01	0.01	0.00	0.00	0.00	0.00		
0.00	0.00									
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
13	1	0.00	0.01	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
14	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
15	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
16	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
17	1	0.00	0.00	0.01	0.00	-0.01	0.00	0.00		
0.01	-0.01									
18	6	0.00	0.01	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
19	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
20	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
21	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
22	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									
23	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
0.00	0.00									

```
    24   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    25   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    26   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    27   1     0.00   0.00   0.00     0.00  -0.01   0.00     0.00
0.03  -0.02
    28   6     0.32   0.53  -0.26     0.00   0.00   0.00     0.00
0.00   0.00
    29   6     0.20  -0.37   0.26     0.00   0.00   0.00     0.00
0.00   0.00
    30   8    -0.04   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    31   8    -0.11   0.22  -0.15     0.00   0.00   0.00     0.00
0.00   0.00
    32   8    -0.18  -0.33   0.16     0.00   0.00   0.00     0.00
0.00   0.00
    33   6     0.00   0.00   0.00    -0.01  -0.06  -0.01    -0.02  -
0.02  -0.08
    34   1    -0.01   0.02  -0.02     0.19   0.72   0.51     0.08
0.32   0.21
    35   1     0.00   0.04   0.01    -0.27   0.03  -0.13     0.57  -
0.10   0.25
    36   1     0.00   0.00   0.00     0.20  -0.03  -0.22    -0.46
0.04   0.47
                     91                     92                     93
                      A                      A                      A
 Frequencies --   3148.6018              3174.0057
3180.5815
 Red. masses --      1.1025                 1.0902
1.0874
 Frc consts  --      6.4395                 6.4707
6.4810
 IR Inten    --      7.5264                 2.0931
3.5506
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     2   6     0.00   0.00   0.00    -0.01  -0.08   0.03     0.00  -
0.02   0.01
     3   1     0.00   0.00   0.00     0.07   0.88  -0.40     0.02
0.20  -0.09
     4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     7   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
```

This journal is © The Royal Society of Chemistry 2014

8	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	1	0.00	0.00	0.00	0.02	-0.02	0.00	0.01	-0.01	0.00
10	6	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
11	1	0.00	0.00	0.00	0.00	-0.06	0.03	0.00	-0.03	0.01
12	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	1	0.00	0.00	0.00	0.02	0.00	-0.01	0.01	0.00	-0.01
14	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	1	-0.01	0.01	0.00	-0.01	0.01	0.00	0.00	0.00	0.00
16	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	1	0.00	-0.04	0.02	0.00	0.00	0.00	0.00	0.00	0.00
18	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	6	0.00	0.00	0.00	0.00	0.02	-0.01	0.00	-0.06	0.03
21	1	0.00	0.00	0.00	-0.02	-0.19	0.09	0.06	0.74	-0.37
22	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.03	0.02	-0.01
23	1	0.00	0.00	0.00	-0.06	0.04	-0.01	0.37	-0.24	0.08
24	6	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.01	0.00
25	1	-0.01	0.00	0.00	0.02	0.01	-0.01	-0.20	-0.08	0.06
26	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.00
27	1	0.00	0.05	-0.02	0.00	-0.01	0.00	0.01	0.06	-0.03
28	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
31	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
33	6	0.09	-0.01	-0.02	0.00	0.00	0.00	0.00	0.00	0.00

```
    34   1     0.02  -0.01  -0.01     0.00   0.00   0.00     0.00
0.00   0.00
    35   1    -0.63   0.10  -0.31     0.00   0.00   0.00     0.00
0.00   0.00
    36   1    -0.47   0.05   0.51     0.00   0.00   0.00     0.01
0.00  -0.01
                     94                     95                     96
                      A                      A                      A
 Frequencies --  3188.7021              3191.8670
3197.2558
 Red. masses --     1.0862                 1.0889
1.0899
 Frc consts  --     6.5071                 6.5362
6.5641
 IR Inten    --     0.1253                 7.3022
8.2246
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     2   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     3   1     0.00   0.06  -0.02     0.00   0.04  -0.02     0.00
0.04  -0.02
     4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     7   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     9   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    10   6     0.00  -0.04   0.02     0.00   0.00   0.00     0.00  -
0.05   0.03
    11   1     0.03   0.50  -0.24     0.00   0.00   0.00     0.04
0.61  -0.29
    12   6     0.04   0.01  -0.03     0.00   0.00   0.00     0.00
0.00   0.00
    13   1    -0.46  -0.13   0.38    -0.01   0.00   0.01    -0.03  -
0.01   0.03
    14   6    -0.03   0.03   0.01     0.00   0.00   0.00     0.04  -
0.04  -0.01
    15   1     0.38  -0.36  -0.09     0.02  -0.01   0.00    -0.49
0.46   0.12
    16   6     0.00  -0.01   0.01     0.00   0.00   0.00     0.00
0.02  -0.01
    17   1     0.00   0.14  -0.07     0.00   0.01   0.00    -0.01  -
0.23   0.12
```

```
    18   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    19   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    20   6     0.00   0.00   0.00     0.00  -0.03   0.02     0.00
0.00   0.00
    21   1     0.00   0.00   0.00     0.03   0.37  -0.18     0.00
0.01   0.00
    22   6     0.00   0.00   0.00     0.03  -0.01   0.00     0.00
0.00   0.00
    23   1     0.02  -0.01   0.00    -0.28   0.17  -0.06     0.00
0.00   0.00
    24   6     0.00   0.00   0.00    -0.06  -0.02   0.02     0.00
0.00   0.00
    25   1    -0.02  -0.01   0.01     0.71   0.29  -0.20     0.01
0.00   0.00
    26   6     0.00   0.00   0.00     0.00   0.02  -0.01     0.00
0.00   0.00
    27   1     0.00   0.01   0.00    -0.02  -0.25   0.13     0.00
0.00   0.00
    28   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    29   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    30   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    31   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    32   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    33   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    34   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    35   1    -0.01   0.00   0.00    -0.01   0.00   0.00     0.01
0.00   0.01
    36   1     0.00   0.00   0.00    -0.02   0.00   0.02     0.00
0.00   0.00
                     97                     98                     99
                      A                      A                      A
 Frequencies --  3206.2884              3210.2791
3217.9693
 Red. masses --     1.0937                 1.0947
1.0941
 Frc consts  --     6.6244                 6.6470
6.6750
 IR Inten    --    22.6624                19.3243
18.3570
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
```

```
     2   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     3   1     0.00  -0.01   0.01     0.00   0.02  -0.01     0.00
0.00   0.00
     4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     6   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     7   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     8   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     9   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    10   6     0.00   0.00   0.00     0.00  -0.04   0.02     0.00
0.00   0.00
    11   1     0.00   0.00   0.00     0.02   0.41  -0.20     0.00
0.00   0.00
    12   6     0.00   0.00   0.00    -0.05  -0.01   0.04     0.00
0.00   0.00
    13   1     0.01   0.00  -0.01     0.57   0.16  -0.47     0.01
0.00  -0.01
    14   6     0.00   0.00   0.00    -0.02   0.02   0.00     0.00
0.00   0.00
    15   1     0.01  -0.01   0.00     0.19  -0.19  -0.04     0.02  -
0.02   0.00
    16   6     0.00   0.00   0.00     0.00  -0.03   0.01     0.00
0.00   0.00
    17   1     0.00   0.01   0.00     0.01   0.33  -0.17     0.00  -
0.05   0.02
    18   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    19   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    20   6     0.00   0.02  -0.01     0.00   0.00   0.00     0.00
0.01   0.00
    21   1    -0.02  -0.26   0.13     0.00   0.01   0.00    -0.01  -
0.07   0.03
    22   6    -0.06   0.04  -0.01     0.00   0.00   0.00    -0.02
0.01   0.00
    23   1     0.66  -0.41   0.15    -0.01   0.01   0.00     0.19  -
0.12   0.04
    24   6    -0.03  -0.01   0.01     0.00   0.00   0.00    -0.04  -
0.01   0.01
    25   1     0.30   0.13  -0.09     0.00   0.00   0.00     0.40
0.16  -0.11
    26   6     0.00   0.03  -0.02     0.00   0.00   0.00     0.00  -
0.07   0.03
    27   1    -0.03  -0.37   0.18     0.00   0.01   0.00     0.06
0.76  -0.38
```

```
    28   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    29   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    30   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    31   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    32   8     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    33   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    34   1     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    35   1    -0.01   0.00   0.00    -0.02   0.00  -0.01     0.01
0.00   0.00
    36   1    -0.02   0.00   0.02     0.00   0.00   0.00     0.04
0.00  -0.04
                     100                    101                    102
                      A                      A                      A
 Frequencies --  3221.0166              3234.0233
3269.2446
 Red. masses --     1.0943                 1.0919
1.0953
 Frc consts  --     6.6893                 6.7284
6.8970
 IR Inten    --    12.4287                 1.0789
0.6501
  Atom  AN      X      Y      Z        X      Y      Z        X      Y
Z
     1   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     2   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     3   1     0.00   0.00   0.00     0.00   0.03  -0.01     0.00
0.00   0.00
     4   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     5   6     0.00   0.00   0.00     0.00   0.00   0.00     0.00
0.00   0.00
     6   6     0.00   0.00   0.00    -0.01   0.00   0.01    -0.06  -
0.03   0.05
     7   1     0.00   0.00   0.00     0.14   0.05  -0.11     0.73
0.29  -0.58
     8   6     0.00   0.00   0.00     0.06  -0.06   0.00    -0.01
0.01   0.00
     9   1     0.00   0.00   0.00    -0.66   0.72   0.06     0.12  -
0.13  -0.01
    10   6     0.00   0.01   0.00     0.00   0.00   0.00     0.00
0.00   0.00
    11   1     0.00  -0.09   0.04     0.00   0.00   0.00     0.00
0.00   0.00
```

This journal is © The Royal Society of Chemistry 2014

12	6	0.01	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
13	1	-0.16	-0.05	0.13	0.00	0.00	0.00	0.00	0.00	0.00
14	6	0.03	-0.02	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
15	1	-0.29	0.28	0.07	0.00	0.00	0.00	0.00	0.00	0.00
16	6	0.00	-0.07	0.04	0.00	0.00	0.00	0.00	0.00	0.00
17	1	0.03	0.78	-0.40	0.00	0.00	0.00	0.00	0.00	0.00
18	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	1	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
22	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	1	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
25	1	0.02	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
26	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	1	0.00	0.05	-0.02	0.00	0.00	0.00	0.00	0.00	0.00
28	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
31	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
32	8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
33	6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
34	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
35	1	-0.03	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
36	1	-0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00

This journal is © The Royal Society of Chemistry 2014

```
 - Thermochemistry -
 -------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Atom     1 has atomic number  6 and mass  12.00000
 Atom     2 has atomic number  6 and mass  12.00000
 Atom     3 has atomic number  1 and mass   1.00783
 Atom     4 has atomic number  6 and mass  12.00000
 Atom     5 has atomic number  6 and mass  12.00000
 Atom     6 has atomic number  6 and mass  12.00000
 Atom     7 has atomic number  1 and mass   1.00783
 Atom     8 has atomic number  6 and mass  12.00000
 Atom     9 has atomic number  1 and mass   1.00783
 Atom    10 has atomic number  6 and mass  12.00000
 Atom    11 has atomic number  1 and mass   1.00783
 Atom    12 has atomic number  6 and mass  12.00000
 Atom    13 has atomic number  1 and mass   1.00783
 Atom    14 has atomic number  6 and mass  12.00000
 Atom    15 has atomic number  1 and mass   1.00783
 Atom    16 has atomic number  6 and mass  12.00000
 Atom    17 has atomic number  1 and mass   1.00783
 Atom    18 has atomic number  6 and mass  12.00000
 Atom    19 has atomic number  6 and mass  12.00000
 Atom    20 has atomic number  6 and mass  12.00000
 Atom    21 has atomic number  1 and mass   1.00783
 Atom    22 has atomic number  6 and mass  12.00000
 Atom    23 has atomic number  1 and mass   1.00783
 Atom    24 has atomic number  6 and mass  12.00000
 Atom    25 has atomic number  1 and mass   1.00783
 Atom    26 has atomic number  6 and mass  12.00000
 Atom    27 has atomic number  1 and mass   1.00783
 Atom    28 has atomic number  6 and mass  12.00000
 Atom    29 has atomic number  6 and mass  12.00000
 Atom    30 has atomic number  8 and mass  15.99491
 Atom    31 has atomic number  8 and mass  15.99491
 Atom    32 has atomic number  8 and mass  15.99491
 Atom    33 has atomic number  6 and mass  12.00000
 Atom    34 has atomic number  1 and mass   1.00783
 Atom    35 has atomic number  1 and mass   1.00783
 Atom    36 has atomic number  1 and mass   1.00783
 Molecular mass:   290.09429 amu.
 Principal axes and moments of inertia in atomic units:
                           1         2         3
     Eigenvalues --  4023.20402  6671.00957  6846.02539
           X            0.99944  -0.02387  -0.02350
           Y            0.01602   0.95668  -0.29071
           Z            0.02942   0.29017   0.95652
 This molecule is an asymmetric top.
 Rotational symmetry number  1.
 Warning -- assumption of classical behavior for rotation
           may cause significant error
 Rotational temperatures (Kelvin)      0.02153     0.01298     0.01265
 Rotational constants (GHZ):           0.44858     0.27053     0.26362
```

This journal is © The Royal Society of Chemistry 2014

```
   1 imaginary frequencies ignored.
 Zero-point vibrational energy     734014.7 (Joules/Mol)
                                  175.43373 (Kcal/Mol)
 Warning -- explicit consideration of  27 degrees of freedom as
          vibrations may cause significant error
 Vibrational temperatures:     76.73   109.11   121.19   142.10
190.93
          (Kelvin)            206.11   218.80   257.53   262.66
307.90
                              346.13   400.93   472.48   482.05
533.04
                              568.50   595.74   603.30   615.64
697.02
                              753.86   760.83   792.75   816.84
843.23
                              869.46   892.03   901.13   957.04
1021.92
                             1031.92  1055.64  1092.73  1099.03
1105.27
                             1110.69  1144.75  1200.05  1232.72
1252.73
                             1264.36  1274.94  1275.63  1303.29
1309.58
                             1356.62  1386.62  1393.60  1433.96
1441.22
                             1474.29  1504.42  1512.37  1519.32
1539.51
                             1552.05  1564.09  1585.08  1631.46
1698.07
                             1715.25  1730.71  1759.49  1806.19
1817.32
                             1825.87  1891.54  1917.30  1921.31
1951.54
                             1980.62  2006.63  2033.96  2035.60
2068.26
                             2141.37  2149.20  2174.34  2190.91
2220.66
                             2226.39  2295.83  2314.78  2380.13
2386.99
                             2606.11  2693.68  4367.68  4484.24
4530.13
                             4566.68  4576.14  4587.83  4592.38
4600.13
                             4613.13  4618.87  4629.93  4634.32
4653.03
                             4703.71

 Zero-point correction=                           0.279571
(Hartree/Particle)
 Thermal correction to Energy=                    0.296102
 Thermal correction to Enthalpy=                  0.297046
 Thermal correction to Gibbs Free Energy=         0.236271
```

This journal is © The Royal Society of Chemistry 2014

Sum of electronic and zero-point Energies=	-957.858271
Sum of electronic and thermal Energies=	-957.841740
Sum of electronic and thermal Enthalpies=	-957.840796
Sum of electronic and thermal Free Energies=	-957.901572

		E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total		185.807	67.878	127.912
Electronic		0.000	0.000	0.000
Translational		0.889	2.981	42.893
Rotational		0.889	2.981	33.574
Vibrational		184.029	61.916	51.446
Vibration	1	0.596	1.976	4.690
Vibration	2	0.599	1.965	3.996
Vibration	3	0.601	1.960	3.790
Vibration	4	0.604	1.950	3.479
Vibration	5	0.613	1.921	2.906
Vibration	6	0.616	1.910	2.760
Vibration	7	0.619	1.900	2.646
Vibration	8	0.629	1.868	2.339
Vibration	9	0.630	1.864	2.302
Vibration	10	0.644	1.820	2.009
Vibration	11	0.658	1.778	1.799
Vibration	12	0.679	1.713	1.542
Vibration	13	0.712	1.619	1.268
Vibration	14	0.716	1.606	1.236
Vibration	15	0.742	1.533	1.078
Vibration	16	0.762	1.481	0.981
Vibration	17	0.778	1.440	0.912
Vibration	18	0.782	1.428	0.894
Vibration	19	0.789	1.410	0.866
Vibration	20	0.841	1.285	0.698
Vibration	21	0.879	1.197	0.601
Vibration	22	0.884	1.186	0.590
Vibration	23	0.906	1.138	0.542
Vibration	24	0.924	1.101	0.509
Vibration	25	0.943	1.062	0.474
Vibration	26	0.963	1.023	0.442
Vibration	27	0.980	0.990	0.417

		Q	Log10(Q)	Ln(Q)
Total Bot		0.210423-108	-108.676908	-250.237827
Total V=0		0.825580D+20	19.916759	45.860033
Vib (Bot)		0.223296-123	-123.651119	-284.717224
Vib (Bot)	1	0.387486D+01	0.588256	1.354510
Vib (Bot)	2	0.271732D+01	0.434141	0.999646
Vib (Bot)	3	0.244332D+01	0.387980	0.893357
Vib (Bot)	4	0.207846D+01	0.317742	0.731627
Vib (Bot)	5	0.153518D+01	0.186160	0.428650
Vib (Bot)	6	0.141817D+01	0.151730	0.349370
Vib (Bot)	7	0.133258D+01	0.124692	0.287113
Vib (Bot)	8	0.112250D+01	0.050185	0.115556
Vib (Bot)	9	0.109923D+01	0.041090	0.094613

This journal is © The Royal Society of Chemistry 2014

Vib (Bot)	10	0.926616D+00	-0.033100	-0.076216
Vib (Bot)	11	0.814834D+00	-0.088931	-0.204771
Vib (Bot)	12	0.690432D+00	-0.160879	-0.370438
Vib (Bot)	13	0.569537D+00	-0.244478	-0.562931
Vib (Bot)	14	0.555949D+00	-0.254965	-0.587079
Vib (Bot)	15	0.491251D+00	-0.308697	-0.710800
Vib (Bot)	16	0.452685D+00	-0.344204	-0.792559
Vib (Bot)	17	0.425986D+00	-0.370605	-0.853350
Vib (Bot)	18	0.418972D+00	-0.377815	-0.869950
Vib (Bot)	19	0.407874D+00	-0.389474	-0.896796
Vib (Bot)	20	0.343903D+00	-0.463564	-1.067396
Vib (Bot)	21	0.306946D+00	-0.512938	-1.181084
Vib (Bot)	22	0.302773D+00	-0.518883	-1.194772
Vib (Bot)	23	0.284548D+00	-0.545845	-1.256854
Vib (Bot)	24	0.271696D+00	-0.565917	-1.303073
Vib (Bot)	25	0.258421D+00	-0.587672	-1.353164
Vib (Bot)	26	0.245997D+00	-0.609070	-1.402436
Vib (Bot)	27	0.235875D+00	-0.627318	-1.444452
Vib (V=0)		0.876088D+05	4.942548	11.380636
Vib (V=0)	1	0.440699D+01	0.644142	1.483191
Vib (V=0)	2	0.326294D+01	0.513609	1.182628
Vib (V=0)	3	0.299395D+01	0.476245	1.096595
Vib (V=0)	4	0.263775D+01	0.421234	0.969928
Vib (V=0)	5	0.211455D+01	0.325219	0.748844
Vib (V=0)	6	0.200373D+01	0.301840	0.695013
Vib (V=0)	7	0.192329D+01	0.284045	0.654038
Vib (V=0)	8	0.172882D+01	0.237750	0.547439
Vib (V=0)	9	0.170761D+01	0.232388	0.535093
Vib (V=0)	10	0.155291D+01	0.191146	0.440130
Vib (V=0)	11	0.145601D+01	0.163164	0.375700
Vib (V=0)	12	0.135246D+01	0.131126	0.301929
Vib (V=0)	13	0.125787D+01	0.099637	0.229423
Vib (V=0)	14	0.124772D+01	0.096116	0.221315
Vib (V=0)	15	0.120095D+01	0.079524	0.183111
Vib (V=0)	16	0.117448D+01	0.069846	0.160826
Vib (V=0)	17	0.115686D+01	0.063280	0.145709
Vib (V=0)	18	0.115233D+01	0.061578	0.141788
Vib (V=0)	19	0.114526D+01	0.058904	0.135632
Vib (V=0)	20	0.110685D+01	0.044089	0.101520
Vib (V=0)	21	0.108670D+01	0.036109	0.083145
Vib (V=0)	22	0.108453D+01	0.035240	0.081144
Vib (V=0)	23	0.107530D+01	0.031529	0.072598
Vib (V=0)	24	0.106905D+01	0.028998	0.066771
Vib (V=0)	25	0.106283D+01	0.026465	0.060938
Vib (V=0)	26	0.105724D+01	0.024173	0.055660
Vib (V=0)	27	0.105284D+01	0.022364	0.051496
Electronic		0.100000D+01	0.000000	0.000000
Translational		0.194207D+09	8.288264	19.084433
Rotational		0.485230D+07	6.685947	15.394963

***** Axes restored to original set *****

Center	Atomic	Forces (Hartrees/Bohr)

This journal is © The Royal Society of Chemistry 2014

Number	Number	X	Y	Z
1	6	-0.000003372	0.000001996	-0.000007395
2	6	0.000003984	0.000002700	0.000002696
3	1	-0.000001594	0.000000963	0.000001980
4	6	-0.000000477	-0.000001270	-0.000000567
5	6	0.000003581	-0.000006687	0.000005194
6	6	0.000001310	-0.000007141	-0.000004740
7	1	0.000003893	-0.000002330	0.000001317
8	6	-0.000002659	0.000002349	0.000005369
9	1	0.000003509	-0.000000003	0.000003870
10	6	-0.000001851	-0.000001201	-0.000003449
11	1	-0.000004281	0.000001162	-0.000003436
12	6	-0.000004838	0.000001989	-0.000005976
13	1	-0.000005448	0.000001718	-0.000007433
14	6	-0.000003070	0.000001287	-0.000005000
15	1	-0.000003199	0.000000800	-0.000007998
16	6	-0.000001489	-0.000001285	-0.000004779
17	1	-0.000001431	0.000002821	-0.000006089
18	6	-0.000001323	0.000003512	0.000002833
19	6	-0.000002889	-0.000001111	0.000002982
20	6	0.000000041	0.000000021	0.000004760
21	1	-0.000002954	0.000001246	0.000006663
22	6	-0.000002048	-0.000002251	0.000008243
23	1	-0.000001020	0.000000403	0.000009778
24	6	-0.000000474	0.000001251	0.000007192
25	1	0.000000633	-0.000000203	0.000009026
26	6	0.000001013	0.000000027	0.000005698
27	1	0.000001705	-0.000000421	0.000003788
28	6	0.000000579	-0.000002563	-0.000007875
29	6	0.000001743	-0.000001669	-0.000001730
30	8	0.000002363	-0.000000547	-0.000003939
31	8	0.000005111	-0.000005676	-0.000005188
32	8	0.000001542	0.000001383	-0.000001710
33	6	0.000004293	0.000009902	-0.000002278
34	1	-0.000000315	-0.000002276	-0.000002919
35	1	0.000006760	0.000001174	-0.000000622
36	1	0.000002671	-0.000000069	0.000001735

Cartesian Forces: Max 0.000009902 RMS 0.000003858

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Search for a local minimum.
Step number 1 out of a maximum of 2
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
Eigenvalues --- -0.08123 0.00106 0.00128 0.00172
0.00182

```
     Eigenvalues ---    0.00230   0.00273   0.00402   0.00697
0.00831
     Eigenvalues ---    0.00915   0.00952   0.01277   0.01430
0.01681
     Eigenvalues ---    0.01922   0.02438   0.02595   0.02706
0.02744
     Eigenvalues ---    0.03003   0.03185   0.03469   0.03917
0.04166
     Eigenvalues ---    0.04514   0.05204   0.05351   0.05366
0.05564
     Eigenvalues ---    0.05648   0.05712   0.05815   0.06456
0.06960
     Eigenvalues ---    0.07489   0.08644   0.08828   0.08977
0.09293
     Eigenvalues ---    0.09409   0.10591   0.10768   0.11442
0.11638
     Eigenvalues ---    0.12657   0.13384   0.13480   0.15239
0.15812
     Eigenvalues ---    0.15849   0.17840   0.19641   0.19994
0.20709
     Eigenvalues ---    0.20930   0.22329   0.22860   0.23155
0.25456
     Eigenvalues ---    0.25714   0.26359   0.27222   0.28441
0.28557
     Eigenvalues ---    0.29816   0.31444   0.31909   0.36862
0.42659
     Eigenvalues ---    0.46602   0.49232   0.50024   0.52730
0.57615
     Eigenvalues ---    0.61133   0.63972   0.72113   0.73768
0.74062
     Eigenvalues ---    0.77637   0.80034   0.80369   0.84699
0.85374
     Eigenvalues ---    0.85546   0.86241   0.93734   0.97760
0.97927
     Eigenvalues ---    1.02736   1.07787   1.08550   1.08718
1.10952
     Eigenvalues ---    1.14075   1.21953   1.24792   1.26761
1.27831
     Eigenvalues ---    1.66859   1.76860
 Eigenvalue     1 is  -8.12D-02 should be greater than     0.000000
Eigenvector:
                          Z8        Z2        Z6        Y6        Z5
   1                   0.54724  -0.49479   0.31360   0.29323  -
0.24196
                          Y5        Y8        X2        Y2        Z3
   1                  -0.19179   0.15997  -0.15587  -0.14483  -
0.11316
 Angle between quadratic step and forces=  77.43 degrees.
 Linear search not attempted -- first point.
 TrRot= -0.000028 -0.000016  0.000049  0.000000 -0.000024  0.000000
 MatCor failed.
```

This journal is © The Royal Society of Chemistry 2014

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
X1	1.12720	0.00000	0.00000	0.00018	0.00021	1.12741
Y1	0.34673	0.00000	0.00000	0.00006	0.00005	0.34678
Z1	-2.52980	-0.00001	0.00000	-0.00028	-0.00020	-2.53000
X2	-0.78528	0.00000	0.00000	0.00009	0.00011	-0.78517
Y2	2.17317	0.00000	0.00000	0.00001	0.00000	2.17317
Z2	-1.87689	0.00000	0.00000	-0.00043	-0.00040	-1.87729
X3	-0.63869	0.00000	0.00000	0.00008	0.00012	-0.63857
Y3	4.03573	0.00000	0.00000	0.00004	0.00002	4.03575
Z3	-2.73824	0.00000	0.00000	-0.00038	-0.00035	-2.73859
X4	0.99481	0.00000	0.00000	0.00027	0.00027	0.99508
Y4	-2.04268	0.00000	0.00000	0.00014	0.00012	-2.04256
Z4	-1.29947	0.00000	0.00000	-0.00012	-0.00004	-1.29951
X5	-1.08608	0.00000	0.00000	0.00034	0.00030	-1.08578
Y5	-2.47630	-0.00001	0.00000	0.00026	0.00024	-2.47606
Z5	0.42333	0.00001	0.00000	0.00004	0.00007	0.42339
X6	0.11577	0.00000	0.00000	-0.00054	-0.00065	0.11512
Y6	0.74481	-0.00001	0.00000	-0.00016	-0.00018	0.74464
Z6	3.30704	0.00000	0.00000	-0.00014	-0.00008	3.30696
X7	-1.39707	0.00000	0.00000	-0.00071	-0.00085	-1.39792
Y7	0.15063	0.00000	0.00000	-0.00009	-0.00010	0.15053
Z7	4.54355	0.00000	0.00000	-0.00030	-0.00028	4.54327
X8	0.20427	0.00000	0.00000	-0.00021	-0.00028	0.20399
Y8	2.99446	0.00000	0.00000	-0.00001	-0.00002	2.99443
Z8	1.87622	0.00001	0.00000	0.00013	0.00018	1.87640

This journal is © The Royal Society of Chemistry 2014

X9	-1.14671	0.00000	0.00000	-0.00020	-0.00027	-1.14699
Y9	4.52362	0.00000	0.00000	0.00002	0.00001	4.52363
Z9	2.03859	0.00000	0.00000	-0.00010	-0.00008	2.03851
X10	3.18214	0.00000	0.00000	0.00003	0.00010	3.18224
Y10	0.90790	0.00000	0.00000	-0.00009	-0.00010	0.90780
Z10	-4.13635	0.00000	0.00000	-0.00053	-0.00041	-4.13676
X11	3.28867	0.00000	0.00000	-0.00010	-0.00001	3.28866
Y11	2.75915	0.00000	0.00000	-0.00019	-0.00020	2.75894
Z11	-5.01951	0.00000	0.00000	-0.00077	-0.00064	-5.02015
X12	5.02828	0.00000	0.00000	-0.00012	-0.00004	5.02825
Y12	-0.88923	0.00000	0.00000	-0.00019	-0.00021	-0.88944
Z12	-4.58602	-0.00001	0.00000	-0.00070	-0.00053	-4.58655
X13	6.58779	-0.00001	0.00000	-0.00039	-0.00028	6.58751
Y13	-0.46524	0.00000	0.00000	-0.00036	-0.00038	-0.46562
Z13	-5.85239	-0.00001	0.00000	-0.00110	-0.00089	-5.85328
X14	4.90436	0.00000	0.00000	-0.00005	0.00000	4.90437
Y14	-3.26342	0.00000	0.00000	-0.00012	-0.00014	-3.26355
Z14	-3.38109	0.00000	0.00000	-0.00055	-0.00039	-3.38148
X15	6.36733	0.00000	0.00000	-0.00025	-0.00019	6.36714
Y15	-4.66103	0.00000	0.00000	-0.00025	-0.00027	-4.66130
Z15	-3.73196	-0.00001	0.00000	-0.00084	-0.00064	-3.73260
X16	2.94766	0.00000	0.00000	0.00015	0.00017	2.94782
Y16	-3.82179	0.00000	0.00000	0.00006	0.00004	-3.82174
Z16	-1.73726	0.00000	0.00000	-0.00025	-0.00013	-1.73739
X17	2.89913	0.00000	0.00000	0.00013	0.00012	2.89925
Y17	-5.64804	0.00000	0.00000	0.00007	0.00006	-5.64798

This journal is © The Royal Society of Chemistry 2014

Z17	-0.80698	-0.00001	0.00000	-0.00024	-0.00012	-0.80710
X18	-3.43618	0.00000	0.00000	0.00024	0.00022	-3.43596
Y18	-1.16505	0.00000	0.00000	0.00005	0.00004	-1.16501
Z18	-0.10886	0.00000	0.00000	-0.00017	-0.00020	-0.10906
X19	-3.28480	0.00000	0.00000	0.00013	0.00014	-3.28466
Y19	1.22468	0.00000	0.00000	-0.00004	-0.00006	1.22462
Z19	-1.33114	0.00000	0.00000	-0.00037	-0.00040	-1.33153
X20	-5.49955	0.00000	0.00000	0.00007	0.00009	-5.49946
Y20	2.64198	0.00000	0.00000	-0.00010	-0.00011	2.64186
Z20	-1.76736	0.00000	0.00000	-0.00027	-0.00036	-1.76771
X21	-5.35226	0.00000	0.00000	-0.00005	-0.00002	-5.35227
Y21	4.47967	0.00000	0.00000	-0.00010	-0.00011	4.47955
Z21	-2.67665	0.00001	0.00000	-0.00029	-0.00037	-2.67702
X22	-7.83956	0.00000	0.00000	0.00015	0.00015	-7.83942
Y22	1.68275	0.00000	0.00000	-0.00004	-0.00005	1.68271
Z22	-1.08781	0.00001	0.00000	0.00010	-0.00004	-1.08785
X23	-9.54566	0.00000	0.00000	0.00011	0.00012	-9.54554
Y23	2.75815	0.00000	0.00000	0.00001	0.00000	2.75814
Z23	-1.47482	0.00001	0.00000	0.00040	0.00022	-1.47460
X24	-8.00776	0.00000	0.00000	0.00027	0.00024	-8.00752
Y24	-0.69611	0.00000	0.00000	0.00007	0.00006	-0.69605
Z24	0.09990	0.00001	0.00000	0.00032	0.00018	0.10008
X25	-9.84657	0.00000	0.00000	0.00036	0.00031	-9.84626
Y25	-1.45085	0.00000	0.00000	0.00018	0.00017	-1.45067
Z25	0.61646	0.00001	0.00000	0.00078	0.00060	0.61706
X26	-5.84512	0.00000	0.00000	0.00034	0.00029	-5.84483

This journal is © The Royal Society of Chemistry 2014

Y26	-2.08239	0.00000	0.00000	0.00010	0.00009	-2.08230
Z26	0.61068	0.00001	0.00000	0.00015	0.00006	0.61074
X27	-6.01633	0.00000	0.00000	0.00047	0.00040	-6.01593
Y27	-3.91029	0.00000	0.00000	0.00022	0.00021	-3.91008
Z27	1.52460	0.00000	0.00000	0.00043	0.00033	1.52494
X28	2.92868	0.00000	0.00000	-0.00018	-0.00024	2.92844
Y28	3.65844	0.00000	0.00000	-0.00014	-0.00016	3.65828
Z28	1.61066	-0.00001	0.00000	0.00048	0.00060	1.61125
X29	2.72516	0.00000	0.00000	-0.00062	-0.00074	2.72441
Y29	-0.03074	0.00000	0.00000	-0.00010	-0.00012	-0.03086
Z29	3.82369	0.00000	0.00000	0.00051	0.00062	3.82431
X30	4.35067	0.00000	0.00000	-0.00038	-0.00047	4.35020
Y30	1.68507	0.00000	0.00000	-0.00020	-0.00022	1.68485
Z30	2.59867	0.00000	0.00000	0.00078	0.00093	2.59961
X31	3.56065	0.00001	0.00000	-0.00096	-0.00111	3.55954
Y31	-1.77514	-0.00001	0.00000	-0.00005	-0.00007	-1.77521
Z31	5.02999	-0.00001	0.00000	0.00081	0.00094	5.03094
X32	3.89598	0.00000	0.00000	0.00007	0.00003	3.89601
Y32	5.50532	0.00000	0.00000	-0.00020	-0.00022	5.50510
Z32	0.69942	0.00000	0.00000	0.00063	0.00078	0.70020
X33	-1.09954	0.00000	0.00000	0.00049	0.00041	-1.09913
Y33	-4.83083	0.00001	0.00000	0.00039	0.00037	-4.83046
Z33	2.02712	0.00000	0.00000	0.00019	0.00022	2.02734
X34	-1.53663	0.00000	0.00000	0.00018	0.00013	-1.53650
Y34	-6.50672	0.00000	0.00000	0.00032	0.00030	-6.50642
Z34	0.87860	0.00000	0.00000	0.00040	0.00041	0.87902

```
   X35        0.73912   0.00001   0.00000   0.00064   0.00054
0.73966
   Y35       -5.12838   0.00000   0.00000   0.00039   0.00037  -
5.12801
   Z35        2.92084   0.00000   0.00000  -0.00010  -0.00003
2.92081
   X36       -2.50725   0.00000   0.00000   0.00078   0.00066  -
2.50658
   Y36       -4.71677   0.00000   0.00000   0.00058   0.00057  -
4.71620
   Z36        3.53366   0.00000   0.00000   0.00045   0.00044
3.53410
         Item               Value     Threshold  Converged?
 Maximum Force            0.000010     0.000450     YES
 RMS     Force            0.000004     0.000300     YES
 Maximum Displacement     0.001108     0.001800     YES
 RMS     Displacement     0.000358     0.001200     YES
 Predicted change in Energy=-6.696247D-09
 Optimization completed.
    -- Stationary point found.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

 1\1\GINC-OPT2017\Freq\RB3LYP\6-31+G(d)\C19H14O3\UCN0868\19-Oct-
2012\0\
 \# freq b3lyp/6-31+g(d)
geom=connectivity\\methylanthracenefreq\\0,1\C
 ,0.596488,0.183481,-1.338712\C,-0.415553,1.149994,-0.993208\H,-
0.33797
 8,2.135618,-1.449015\C,0.526431,-1.080941,-0.687648\C,-0.574729,-
1.310
 401,0.224014\C,0.061263,0.394138,1.75001\H,-
0.739299,0.079708,2.404342
 \C,0.108094,1.584598,0.992854\H,-
0.606815,2.393798,1.078775\C,1.683917
 ,0.480442,-2.188863\H,1.740288,1.460079,-2.65621\C,2.660852,-
0.470562,
 -2.426819\H,3.486107,-0.246195,-3.096951\C,2.595277,-1.726925,-
1.78919
 8\H,3.369445,-2.46651,-1.974868\C,1.559833,-2.022403,-
0.91932\H,1.5341
 54,-2.988812,-0.427035\C,-1.818348,-0.616516,-0.057605\C,-
1.73824,0.64
 8072,-0.704407\C,-2.910235,1.398074,-0.935244\H,-2.832292,2.370537,-
1.
 416424\C,-4.148519,0.890475,-0.575642\H,-5.051345,1.459548,-
0.780441\C
 ,-4.237524,-0.368363,0.052865\H,-5.210581,-0.767755,0.326218\C,-
3.0931
 03,-1.101954,0.323158\H,-3.183706,-
2.069235,0.806786\C,1.549792,1.9359
```

64,0.852323\C,1.44209,-
0.016267,2.023409\O,2.302277,0.8917,1.375159\O,
1.884214,-0.939364,2.661757\O,2.061662,2.91329,0.370117\C,-0.581853,-
2
.556366,1.072706\H,-0.81315,-3.443208,0.464937\H,0.391125,-
2.713821,1.
545642\H,-1.326777,-2.496005,1.869933\\Version=AM64L-
G09RevA.01\State=
1-A\HF=-958.1378426\RMSD=4.675e-09\RMSF=3.858e-
06\ZeroPoint=0.2795715\
Thermal=0.2961022\Dipole=-2.1278889,-0.6232028,-
0.8853187\DipoleDeriv=
-0.1108763,-0.0035155,-0.112369,0.0113265,-0.0632177,0.0925181,-
0.1647
886,0.1360453,0.0002438,0.2120266,-0.048802,-0.0793154,-
0.0816826,0.16
80784,-0.0582232,-0.0428631,-
0.0296164,0.1172351,0.0235377,0.01419,0.0
11647,0.006725,-0.017733,0.0359806,0.0116279,0.079959,0.027191,-
0.2044
846,-0.1249004,-0.019917,-0.1690824,-0.17825,0.1434652,-
0.0552936,0.11
11808,0.0100004,0.4574508,-0.0343074,-0.0795225,0.0755204,0.4928696,-
0
.0187923,-0.031556,-0.0642484,0.3331624,-0.6511596,-0.020641,-
0.467291
7,0.2712567,0.037514,0.1654034,-0.2152449,-0.1059879,-
0.3983562,0.0196
668,-
0.0353929,0.0151219,0.0379665,0.0585582,0.0585005,0.0714471,0.020
9133,0.0601286,-0.4734173,-0.2498802,-0.0562599,-0.2124452,-
0.135493,-
0.1693855,0.1967211,0.0372053,0.2040859,0.0216904,0.0172422,-
0.0346795
,0.0239684,-0.0023644,-0.0257124,0.0485583,0.0072979,0.0546685,-
0.0083
073,0.0176526,-0.0100706,0.0479346,0.0653323,-0.1456789,-0.0515691,-
0.
0689103,-0.0798071,0.0696552,0.0345509,0.0172263,-0.0074055,-
0.0358492
,0.0878245,0.0181096,0.0404976,0.0781545,0.0023747,0.061466,-
0.0883911
,0.0979785,-0.0292692,-0.0556238,-0.0981386,-0.0929513,-0.035143,-
0.02
03706,-0.0074072,0.1189444,-
0.0172495,0.0723239,0.0425173,0.1059243,0.
0325038,0.0385317,-0.0192742,-0.1138046,-0.0074893,-
0.142936,0.0747733
,-0.0129048,0.0280125,-0.0117138,-0.1030068,-
0.0107398,0.1007221,0.061
9505,0.1002218,-0.004813,-0.0130428,0.0452217,0.0011399,0.0969657,-
0.0

This journal is © The Royal Society of Chemistry 2014

021765,-0.007089,-0.0251121,-0.0613956,0.0547805,-0.0482239,-
0.0059869
,-0.1049679,-0.090824,0.0734493,-0.0137092,0.0243949,0.0086367,-
0.0292

937,0.0486742,0.0023968,0.0846193,0.07319,0.0644899,0.1060019,0.071634
3,-0.000855,-0.2865569,0.0134645,0.164576,-0.0067718,-
0.0776027,0.1542
061,-0.0030627,0.0903975,0.1272586,-
0.0920518,0.0414185,0.065577,0.050
4046,-0.1728493,-0.0616051,-0.0437808,-0.0789528,-
0.0960367,0.0806794,
-0.1027241,-0.0007723,-0.1107203,-0.0750992,0.0600735,-
0.0425341,0.024
8486,0.0229859,-0.0421858,0.0832744,0.0051035,0.0845265,0.0736687,-
0.0
319247,-0.0739795,0.0390785,-0.0773117,0.039549,-0.0264856,0.037651,-
0
.0899016,-0.1050006,-0.0714128,0.0786789,-
0.0242727,0.0870934,0.036340
6,0.0457384,-0.0276962,0.043628,0.1175851,0.0097786,0.1031201,-
0.03919
11,0.1205227,-0.0283502,-0.0865477,-0.0574772,-0.0425218,-0.0815907,-
0
.0960273,-0.0514209,0.038804,-
0.0630618,0.0566855,0.0423022,0.0477439,
0.0430697,0.1131457,-0.0070453,-0.0390667,-
0.0692953,0.0606098,0.05280
87,-0.0764369,-0.0922111,-0.0617008,-
0.0984465,0.0752243,0.0123679,0.0
010335,-0.0280043,-
0.0403305,0.070377,0.0305762,0.0682046,0.076591,1.2
063145,0.5229347,0.4854152,0.4060134,1.6035139,-0.3349633,-
0.2216403,-
0.693182,0.4054772,1.431953,0.4017381,0.9236769,-
0.3297208,1.0986365,-
1.0019645,0.1747514,-0.6129106,0.86454,-0.734573,-0.1559387,-
0.1813126
,-0.1159285,-1.1012461,0.471972,0.1018556,0.5847402,-0.385804,-
0.69283
89,0.109323,-0.4964913,0.3603043,-0.7038771,0.6799163,-
0.2936816,0.311
9987,-0.8030081,-0.6962038,-0.5049945,-0.0782063,-0.4224537,-
1.1353852
,0.071277,0.1830544,0.3690791,-0.3330267,-0.0236969,0.0235452,-
0.02418
94,-0.0135539,-0.0967302,0.0815214,-0.0495253,-
0.010858,0.0201044,0.06
98585,-0.0474317,-0.0108991,-0.0485962,-0.1017718,-0.0440463,-
0.009195
7,-0.0551642,0.0139201,-0.023015,0.0447454,-0.0450533,-
0.0014605,0.075

8532,-0.0150247,-0.0146682,0.0304558,0.0731859,-0.0126009,-
0.0266201,0
.104109,0.0228567,0.0564715,-0.040365,0.0934005,0.0246577,-
0.0122108\P
olar=296.412116,-8.626727,224.0882489,-13.8990932,-
14.1031264,196.7058
896\PG=C01 [X(C19H14O3)]\NImag=1\\0.53861040,-0.07942087,0.57917980,-
0
.21953556,-0.11669592,0.37235489,-
0.16929208,0.08476708,0.05637413,0.5
3450836,0.08297077,-0.17940682,-0.01052342,-
0.03431938,0.64381526,0.02
328198,0.00731477,-0.06731460,-0.13964530,-
0.17430169,0.18485271,0.004
22285,0.01974605,-0.01122753,-0.05679287,-
0.01454084,0.01467571,0.0573
7305,-0.00220524,-0.01629350,0.00979481,-0.01565314,-
0.28289633,0.1102
1993,0.01645278,0.30053953,-0.00025924,-
0.00906826,0.00565886,0.015332
90,0.11584670,-0.08739218,-0.01608175,-0.11828312,0.09000487,-
0.122064
69,0.00548882,0.02735376,0.01597924,0.01257482,-0.02625655,-
0.00192709
,0.00407984,0.00437551,0.52189142,0.01013523,-
0.23110252,0.06697202,0.
01741557,-0.03313500,-0.00053281,0.00317378,-0.00032720,0.00041400,-
0.
11792396,0.57595603,0.02671669,0.07910514,-0.11888696,-
0.01412353,0.00
679485,0.02208626,0.00223788,-0.00181455,0.00086888,-0.18445534,-
0.131
34070,0.36053807,0.01295045,-0.02782568,0.01049513,-0.02763436,-
0.0002
3095,-0.00159545,-0.00113240,0.00034633,0.00032208,-
0.17119336,0.00038
251,0.08876712,0.52305002,-
0.02965956,0.00444572,0.01898379,0.00171427
,-0.00817011,-0.00835221,0.00047410,0.00047705,0.00044153,-
0.02023266,
-0.10183732,0.04660920,-0.07954536,0.43426505,0.00071184,0.02887185,-
0
.01437281,-0.00238373,-0.01191641,-0.02584393,-0.00001375,-
0.00061388,
-0.00096098,0.07441553,0.03446238,-0.12566753,-0.10317264,-
0.20214831,
0.33580457,0.00050421,-0.00212558,0.00269983,-0.00403982,0.00205138,-
0
.00153382,-0.00007923,-0.00030622,-0.00034417,0.00321636,0.00049788,-
0
.00283938,0.00015999,0.01764142,0.02021129,0.61323947,0.01537685,-
0.01

808352,-0.00744999,0.01694509,0.02433553,0.04784382,-0.00067218,-
0.001
04083,-0.00185215,0.01872774,-0.00170567,-
0.02603800,0.01776918,0.0230
9867,0.04963768,0.01951068,0.38978439,-0.00286176,-0.00003607,-
0.00073
812,-0.00268915,0.00230676,-0.01880746,-0.00037186,-0.00030904,-
0.0012
9036,0.00520266,-0.00363157,-
0.01357547,0.00742995,0.01974956,0.009498
10,-0.15857683,-0.27694352,0.38450697,-0.00066343,0.00086812,-
0.000089
48,0.00036252,-0.00029336,-0.00191842,-0.00003610,-0.00000612,-
0.00010
465,-0.00103676,-0.00018150,0.00063203,0.00011315,-0.00181663,-
0.00365
384,-0.22114094,-0.05844562,0.14139687,0.23037779,-
0.00072769,0.001197
38,-0.00025598,-0.00061075,-0.00192488,-
0.00279694,0.00002802,0.000134
17,0.00022947,-0.00137009,-0.00046041,0.00135127,0.00017325,-
0.0032657
9,-0.00865822,-0.05589515,-
0.06164136,0.06768727,0.06936020,0.06734770
,-0.00108719,0.00146964,-0.00004270,0.00007222,-0.00088138,-
0.00312151
,-0.00007572,-0.00001096,-0.00007793,-0.00168767,-
0.00038746,0.0013006
9,0.00019288,-0.00420766,-0.00971101,0.14975095,0.07600320,-
0.14936160
,-0.14840629,-0.06801236,0.15283303,0.00551907,-
0.00310237,0.00091201,
-0.00773141,0.01047079,0.02991130,-0.00074069,-0.00013247,-
0.00169600,
0.00236061,0.00313433,-0.00136142,-0.00503741,0.00067850,0.00233915,-
0
.09688666,-0.01227401,0.02498496,0.00677420,-
0.02057546,0.00932713,0.5
5910125,-0.00600612,0.00143699,-0.00455748,-0.00382622,-0.02862483,-
0.
00712077,0.00207097,0.00256692,0.00750821,-0.00853628,-
0.00181045,0.00
688296,-0.00585991,-0.01443655,-0.01842260,0.00902079,-
0.24336515,0.13
857969,0.00051964,-0.00309657,-0.00234396,-
0.13890680,0.63834306,0.025
20066,-0.03208387,-0.02637281,0.03095993,0.04134198,0.08156678,-
0.0028
0064,-0.00357889,-0.00818267,0.01449392,0.00427198,-
0.01777307,0.01167
632,0.01273023,0.03260421,0.01435194,0.06726988,-0.12819387,-
0.0020009

This journal is © The Royal Society of Chemistry 2014

4,0.01491790,0.00054670,-0.06733056,-0.13485178,0.13980560,-
0.00168021
,0.00082608,-0.00014991,0.00053094,-0.00411457,-
0.00481256,0.00029156,
0.00010199,0.00067052,-0.00102125,-0.00055702,0.00100615,0.00057821,-
0
.00150437,-0.00131484,0.00726310,-0.00192990,-0.00149689,-
0.00004341,-
0.00002539,-0.00102500,-0.18345846,0.14652583,0.02504306,0.19090297,-
0
.00107091,0.00079485,0.00000268,0.00019045,-0.00412164,-
0.00568817,0.0
0012337,0.00066830,0.00038140,-0.00090624,-
0.00019799,0.00070902,0.000
42222,-0.00068074,-0.00038289,0.01584095,-0.00733947,-0.00431283,-
0.00
064356,0.00055091,-0.00046110,0.15290542,-0.21918794,-0.00470824,-
0.15
909419,0.22255596,-0.00335112,0.00251382,-0.00015385,0.00123030,-
0.013
97490,-0.01568400,0.00058556,0.00040286,0.00048206,-0.00209885,-
0.0010
2697,0.00190066,-0.00020974,-0.00215843,-0.00419391,-
0.01444199,0.0183
7843,0.00236466,-0.00038022,-0.00228695,-0.00128920,0.02990208,-
0.0172
7037,-0.02198826,-0.01697147,0.01225196,0.03822095,-0.19605798,-
0.0176
5141,0.09953827,-0.03522996,0.01217687,0.03267201,0.00070995,-
0.002242
09,-0.00147913,0.02358845,-0.04500020,0.01141903,-
0.00273468,0.0036860
8,0.00708072,0.00034608,-
0.01046300,0.00155773,0.00039308,0.00045907,0
.00067411,-0.00304420,0.00433573,-
0.01632943,0.00076626,0.00063784,0.0
0183649,0.51734999,-0.04632693,-
0.12618260,0.05475070,0.02283966,0.008
78427,-0.01580712,0.00035927,0.00066121,-0.00148719,-
0.02825868,0.0063
6271,0.01898120,0.00258631,-0.00602219,0.00263244,-
0.00022438,0.001370
10,-0.00100275,-0.00011275,-0.00016280,-0.00022336,-0.00036284,-
0.0010
1750,0.00110326,-0.00002935,-0.00009817,-0.00025145,-
0.11969635,0.6823
7100,0.11353591,0.03455889,-0.15331495,0.01479557,-0.00678870,-
0.00922
008,-0.00159108,0.00028664,-0.00075770,0.00222224,0.03304050,-
0.012294
06,0.00226488,0.00270565,0.00093564,-0.00033005,0.00414582,-
0.00054317

,-0.00015021,-0.00012682,-0.00029616,0.00129339,-
0.00174416,0.00655385
,-0.00022236,-0.00023976,-0.00079918,-0.20978210,-
0.15970176,0.3470407
8,0.00121243,-0.02195357,0.01095316,0.00060916,-0.00234287,-
0.00128981
,-0.00026680,0.00072299,-0.00009550,-
0.00201769,0.00124000,0.00475931,
0.00056558,-0.00138450,0.00034166,-0.00003773,-0.00005064,-
0.00001610,
-0.00000701,0.00000825,-0.00000101,0.00008839,-0.00005630,-
0.00013663,
-0.00001677,0.00000781,-0.00001283,-0.05375680,-
0.00951711,0.01578332,
0.05124512,0.00041032,-0.00287842,0.00236354,0.00055149,0.00024668,-
0.
00167229,-0.00037267,0.00046826,0.00029223,-
0.00017159,0.00187166,0.00
130068,0.00061136,-0.00032631,-
0.00027142,0.00004765,0.00010483,0.0000
6461,0.00000511,0.00001050,-
0.00000031,0.00014441,0.00002003,0.0001570
5,-0.00000817,-0.00000574,-0.00004958,-0.00877877,-
0.28392597,0.115188
85,0.00788253,0.29949652,-0.00008857,0.01778572,-0.00476299,-
0.0023126
0,-0.00035309,-0.00139220,0.00052432,-
0.00047488,0.00003619,0.00504407
,0.00076840,0.00207617,-0.00019535,0.00112902,-0.00017814,-
0.00015943,
0.00008556,-0.00007855,-0.00002557,-0.00002300,-
0.00000208,0.00009126,
-0.00025353,-0.00019405,-0.00004301,-0.00004042,-
0.00007430,0.01662714
,0.11469769,-0.09785868,-0.02089194,-0.12605071,0.09439731,-
0.04286070
,0.00938136,0.02966418,0.00376986,-0.00647585,-
0.00157110,0.00002121,0
.00021416,-0.00014467,-0.01206429,0.01487656,-0.00443250,0.00214972,-
0
.00072160,-0.00378518,0.00021717,0.00428165,0.00035353,-0.00007944,-
0.
00005602,-0.00018915,0.00087221,-0.00210343,0.00593328,-0.00018010,-
0.
00020398,-0.00072387,-0.22892086,0.15331038,0.04800075,0.00552275,-
0.0
0310223,-0.00012798,0.57520693,0.04160467,0.02944504,-0.03605593,-
0.01
078606,0.01064094,0.01508849,-0.00028650,-
0.00013248,0.00006749,0.0282
5475,-0.04044297,-0.00104186,-0.00739714,0.00166125,0.00916331,-
0.0003

2148,-0.01051518,0.00017000,0.00041374,0.00058060,0.00077243,-
0.001480
07,0.00437289,-
0.01236335,0.00058514,0.00051967,0.00137768,0.10392055,
-0.23560464,0.00422560,0.02152433,-0.01476688,-0.00582876,-
0.10481339,
0.59469723,0.01256354,-0.01764628,0.00324466,0.00619672,0.00226838,-
0.
00061772,0.00002609,-0.00020579,0.00005960,-0.00824740,0.00499842,-
0.0
0315781,0.00109588,-0.00042200,-0.00206068,0.00017330,0.00211740,-
0.00
050132,-0.00016272,-0.00028322,-0.00024121,-
0.00007305,0.00004539,0.00
247677,-0.00002193,-0.00005996,0.00004141,0.06986455,-0.02600735,-
0.09
570001,-0.01072264,0.01038462,0.00650141,-0.25678981,-
0.14197018,0.376
50835,0.00079985,0.00528044,0.00299176,-0.00047442,-
0.00090716,0.00030
731,0.00000883,0.00005609,0.00009237,-0.00016158,0.00007217,-
0.0003925
0,-0.00002445,-0.00019978,-
0.00046641,0.00007297,0.00016166,0.00002354
,-0.00000489,-0.00001981,-0.00001265,0.00006439,-
0.00005933,0.00018902
,-0.00001103,-0.00001117,-0.00002036,-0.01289728,-
0.00605178,0.0142375
3,-0.00054345,-0.00086351,-0.00236624,-0.21582671,-
0.04009028,0.140925
97,0.22412438,0.00430619,-
0.00207316,0.00116510,0.00074196,0.00072923,
-0.00029090,-0.00001812,-0.00001290,0.00003454,0.00058832,-
0.00106925,
-0.00010129,-0.00022434,-0.00004386,-0.00019816,-0.00001402,-
0.0000730
2,-0.00000731,0.00000192,0.00000165,0.00000847,-
0.00005195,0.00000773,
-0.00007602,-0.00000030,0.00000745,0.00001590,0.01758443,0.00898006,-
0
.01445636,-0.00132847,0.00031967,-0.00127158,-0.04005785,-
0.06941195,0

.04250440,0.04102170,0.06759655,0.00294730,0.00133512,0.00534624,0.000
19381,0.00009363,-0.00001194,0.00001330,0.00001656,0.00010724,-
0.00078
429,-0.00044086,0.00006106,-0.00014592,-0.00023321,-0.00062475,-
0.0000
3056,0.00020482,-0.00000427,-0.00001686,-0.00000608,-0.00000476,-
0.000
01359,-0.00021816,0.00021105,-0.00003677,-0.00002038,-
0.00004299,0.003

03368,0.00244743,0.00059857,-0.00208051,-0.00155588,-
0.00240648,0.1409
9544,0.04181851,-0.15340932,-0.15525670,-0.04780609,0.15417087,-
0.0171
2687,-0.01273420,0.01192042,0.00260398,-0.00404371,-
0.00441833,0.00009
411,0.00003995,-0.00006242,-
0.04397964,0.02557975,0.02218098,0.0062434
3,0.00267485,-0.00627383,0.00079473,0.00587541,0.00065145,-
0.00018050,
-0.00039943,-0.00045137,0.00044497,-0.00208420,0.00525203,-
0.00020452,
-0.00022345,-0.00044103,0.02901910,0.01437461,-0.02041870,-
0.00106040,
0.00476667,0.00385158,-0.11038243,0.03001041,0.01911053,0.00284057,-
0.
02289130,0.01088121,0.56855853,-0.02427314,-
0.01506241,0.01960065,0.00
451181,-0.00573172,-0.00655504,0.00004330,0.00023353,-0.00016875,-
0.00
747547,0.03655392,-0.01304709,0.01214950,-0.00587137,-
0.00709547,0.000
55930,0.00746132,0.00173421,-0.00023558,-0.00025705,-
0.00044217,0.0010
2751,-0.00394570,0.00736172,-0.00048092,-0.00033849,-
0.00114010,0.0475
1650,-0.04392582,-0.00758746,0.00393312,-0.00006206,0.00080414,-
0.0195
6974,-0.26332286,0.10843575,0.00119588,-0.00105260,0.00124373,-
0.13583
087,0.61241950,0.02019293,0.01327898,-0.02433156,-
0.00474831,0.0053064
3,0.00560073,-0.00007665,-0.00014228,-0.00006276,0.03637832,-
0.0310594
1,-0.00270639,-0.00655665,0.00321107,0.01268466,-0.00059899,-
0.0073576
2,-0.00045234,0.00032531,0.00048339,0.00057469,-
0.00066335,0.00312694,
-0.00709424,0.00034127,0.00034490,0.00079019,-
0.03842451,0.01385353,0.
02536358,0.00418331,0.00010262,0.00482897,0.04248708,0.07403944,-
0.126
48035,-0.00032007,0.01761442,-0.00492970,-0.23959763,-
0.13387121,0.363
98821,-0.00028886,-0.00037460,-0.00010752,0.00000004,-0.00027125,-
0.00
051883,-0.00000958,0.00003377,-0.00000029,0.00019365,-
0.00086563,0.006
29251,-0.00023180,0.00092267,-
0.00056405,0.00007611,0.00018843,0.00008
286,-0.00000558,-0.00000442,-0.00001589,0.00008724,-
0.00008868,0.00017

769,-0.00000755,-0.00000259,-
0.00003549,0.00268049,0.00008732,0.002139
29,0.00011261,-0.00018786,0.00009332,0.00485575,-
0.00262849,0.00007537
,-0.00032316,-0.00046084,-0.00174386,-
0.19579700,0.14048191,0.04331957
,0.20279730,-0.00104340,0.00004649,0.00026296,0.00006964,-
0.00019266,-
0.00042637,-0.00003189,0.00003921,0.00001230,-
0.00025704,0.00162189,0.
00352932,-0.00013451,0.00032488,-0.00008439,-0.00003588,0.00023840,-
0.
00008258,-0.00001895,-0.00001375,-0.00002616,0.00003405,-
0.00008882,0.
00024244,-0.00002019,-0.00001156,-0.00002789,-0.00049627,-
0.00324799,0
.00466293,0.00107511,-0.00078115,-0.00031120,0.02118453,-0.01428107,-
0
.00642205,-0.00101164,0.00048353,-0.00102501,0.14065063,-0.18715158,-
0
.02624383,-0.15263478,0.19458177,0.00000292,0.00066706,-0.00092906,-
0.
00027306,-0.00041127,-0.00051897,0.00005348,-
0.00002507,0.00000723,0.0
0527553,0.00340767,0.00234717,0.00076869,-0.00060537,0.00043027,-
0.000
09569,0.00015502,-0.00006613,-0.00001032,-0.00000224,-
0.00000423,0.000
03818,-0.00006361,0.00012091,-0.00001528,-0.00000485,-
0.00002152,0.002
69590,0.00409736,0.00210751,-0.00054077,0.00058117,0.00026419,-
0.01135
953,0.01030779,0.00601956,-0.00145238,-0.00144474,-
0.00154135,0.043158
15,-0.02576954,-0.05471396,-
0.05050474,0.02553679,0.04847403,0.0303428
3,0.03011483,-0.02847648,-
0.00335947,0.00468839,0.00971185,0.00036875,
-0.00074489,-0.00017113,-0.17656385,0.08621884,0.03712896,-
0.03837122,
0.01870838,0.02549827,-0.00199135,-0.01217202,-
0.00250373,0.00053891,0
.00077538,0.00090028,-0.00086749,0.00557103,-
0.00891506,0.00057516,0.0
0047738,0.00125829,-0.04452036,0.01344633,0.01987651,-
0.00090053,0.000
11274,0.00021236,0.02096451,-
0.06219530,0.01893326,0.00275463,0.001724
98,0.00141319,-0.24305886,0.00075385,0.12903903,-0.01303776,-
0.0063954
7,0.01451734,0.51686467,0.01404519,-
0.03575211,0.00853712,0.00027191,-

0.00448740,0.00295738,0.00087684,-0.00081548,-0.00055459,0.11157428,-
0
.19754038,-0.00556216,0.00332413,0.00895207,-
0.01038187,0.00113892,0.0
0398768,0.00106286,-0.00018513,-0.00027237,-0.00034511,-0.00007529,-
0.
00104351,0.00289941,-0.00011018,-0.00012599,-0.00013042,0.01109790,-
0.
00509406,-0.00636300,0.00017485,0.00035675,-0.00040928,-
0.02712891,0.0
0408427,0.02083992,0.00099513,-0.00414129,0.00408156,-0.04724412,-
0.12
985361,0.06649206,0.01729265,0.00841584,-0.01475402,-
0.07951523,0.6345
5453,-0.02295731,-0.00422209,0.02302646,0.00366220,0.00299853,-
0.00133
836,-0.00059731,0.00093854,0.00043375,0.02795171,0.01129826,-
0.0909965
0,0.02230920,-0.01627773,-0.00503506,-
0.00001597,0.00340866,0.00006841
,-0.00012771,-0.00028869,-0.00028931,0.00003811,-
0.00185893,0.00253892
,-0.00020392,-0.00025879,-0.00041145,0.02148487,-0.00874702,-
0.0141897
3,0.00005060,-0.00048691,-0.00062324,0.00394544,0.04253867,-
0.01557044
,0.00161621,0.00351766,0.00304439,0.15332240,0.03559395,-
0.18542525,0.
00335623,0.00220181,0.00055138,-0.23003386,-0.19300641,0.38921256,-
0.0
0208903,0.00342944,0.00357938,0.00065209,0.00094661,-0.00088389,-
0.000
23178,0.00030268,0.00026749,0.00388743,0.02023626,-
0.01078492,0.000678
72,-0.00009215,-0.00175537,-0.00003070,-0.00010518,-0.00013955,-
0.0000
1134,0.00001941,0.00002759,-0.00003297,0.00002933,-0.00002607,-
0.00000
101,-0.00002423,0.00000470,-0.00089123,0.00008565,0.00006435,-
0.000168
47,-0.00023830,-0.00055468,-
0.00118835,0.00119721,0.00583109,0.0000191
9,-0.00108099,0.00055316,0.00333834,-0.02277991,0.01159379,-
0.00059601
,-0.00090543,-0.00247509,-0.05273518,-
0.00062151,0.01161687,0.05127586
,0.00412510,0.00036117,-0.00024081,-0.00044311,-
0.00072468,0.00084265,
0.00025793,-0.00022364,-0.00007370,-0.00152162,-
0.01462612,0.00947643,
-0.00166719,-0.00071602,0.00029054,-0.00013889,-0.00003720,-
0.00024214

,-0.00000889,-0.00001644,-0.00002217,-0.00002083,-
0.00002370,0.0000525
8,-0.00001982,-0.00000232,-0.00001821,0.00017615,0.00014765,-
0.0005781
9,-0.00029101,-0.00020582,-
0.00029223,0.00050031,0.00252956,0.00247972
,0.00016065,-0.00016643,0.00006068,0.00116679,-
0.00196270,0.00203664,-
0.00131559,0.00015152,-0.00157345,-0.00024318,-
0.28207579,0.12119002,0
.00024137,0.29606624,0.00255104,0.00052163,0.00311155,0.00029161,-
0.00
043858,0.00009283,0.00011656,-0.00006992,0.00011975,-0.00127636,-
0.005
03107,0.00624297,-0.00072737,-0.00054922,-
0.00204526,0.00002597,0.0000
7720,-0.00012872,-0.00002486,-0.00002946,-0.00002924,-0.00000419,-
0.00
003285,0.00018375,-0.00000365,-0.00001750,-0.00001149,0.00022323,-
0.00
071181,-0.00047349,-0.00050726,-0.00024222,-
0.00065929,0.00623564,0.00
179365,0.00266426,-0.00002085,0.00092811,-0.00029767,-
0.00042460,0.018
76002,-0.00482822,-0.00228626,-0.00177930,-
0.00228468,0.01267051,0.120
96803,-0.10329300,-0.01875763,-0.13381668,0.10337990,-
0.00485051,0.006
32151,-0.00472032,0.01950444,-0.02459031,0.02275650,-0.00592002,-
0.002
33925,-0.00052495,-0.04069058,0.00492329,0.00385396,-
0.19148301,0.0743
1172,-0.00718398,-0.01156996,-0.02516972,-
0.01041853,0.00054556,0.0018
9363,0.00222310,-0.00135512,0.00808282,-
0.01666784,0.00038655,0.000658
32,0.00150130,0.00147057,-0.00030442,-0.00113347,0.00007753,-
0.0000602
7,-0.00020245,-0.00062737,0.00277754,-
0.00044996,0.00004155,0.00001366
,0.00004262,-0.00189866,-0.00151558,0.00308200,-0.00037318,-
0.00020799
,-0.00009029,0.00543605,-0.00383008,0.00075172,-0.00028113,-
0.00003201
,-0.00042557,0.65355722,0.00704440,-0.00922402,0.00094008,-
0.03351327,
-0.01617475,0.00250483,-
0.00015897,0.00188431,0.00253261,0.01246017,0.
01312392,-0.01070504,0.04886572,-0.12924298,0.03726694,-
0.00004324,0.0
0711329,-0.00132342,-0.00108066,-0.00108819,-0.00148860,-0.00272463,-
0

.00418225,0.01100984,0.00034675,-0.00057851,-0.00079217,-
0.00350542,0.
00047143,0.00126875,0.00007312,0.00017293,-0.00004977,0.00153222,-
0.00

362231,0.00051286,0.00006183,0.00000086,0.00008711,0.00206136,0.003966
29,-0.00326626,-0.00029285,-0.00012742,-0.00017397,-
0.00613050,0.00253
040,0.00586654,-
0.00018032,0.00023714,0.00022524,0.00077423,0.52708838
,-0.00145437,0.00112212,-
0.00170236,0.01271736,0.01120194,0.00104347,0
.00094622,0.00045377,0.00257962,0.01889600,-0.01195448,0.00448777,-
0.0
1769050,0.04297137,-0.07249781,-0.00884786,-0.01113822,-0.00906689,-
0.
00177863,-0.00019502,0.00014369,-0.00342724,0.00176414,-
0.00629552,0.0
0027157,0.00058182,0.00118457,-0.00016620,-0.00021463,-
0.00028553,0.00
005951,-0.00001824,-0.00007986,0.00063489,-
0.00032273,0.00003909,0.000
02587,0.00005774,0.00002474,0.00075613,-0.00014169,-
0.00088273,0.00015
602,-0.00007763,-0.00051577,0.00272261,0.00370520,-0.00056082,-
0.00009
296,-0.00008351,0.00012502,-0.04860508,-0.19342641,0.27519430,-
0.03892
407,0.00517227,0.00099122,-0.22398241,-
0.05132486,0.06431084,0.0014719
0,0.00013264,-0.00132539,-0.00594047,-
0.00704596,0.00315429,0.02663138
,0.02676361,-0.00734588,-0.00270317,-
0.01936351,0.00167672,0.00024617,
0.00081003,0.00120382,-0.01441345,0.00301714,-
0.04058862,0.00089785,0.
00152063,0.00387325,0.00500713,0.00157212,-0.00256935,-0.00027395,-
0.0
0041571,-0.00017715,-0.00120939,0.00334258,0.00041199,-
0.00021984,0.00
006370,-0.00015805,-0.00111195,-0.00208824,0.00194792,0.00003918,-
0.00
001570,0.00003868,0.00211399,-0.00112279,-0.00080773,0.00010626,-
0.000
15104,-0.00014738,-0.13546222,-
0.00886433,0.01720416,0.67810712,0.0156
9161,0.01717480,-0.00707360,-0.04798372,-0.12286597,0.03841976,-
0.0266
0552,-0.00708176,0.00343786,-0.00556718,-
0.00391774,0.00350383,0.02763
667,-0.01770881,0.01441635,-0.00163580,-0.00869923,-0.00070727,-
0.0000

0917,0.00074262,0.00115006,-0.00723586,-0.00030941,-0.01578181,-
0.0014
5997,0.00041229,0.00060703,0.00440150,-0.00458024,-
0.00073136,0.000161
18,0.00003968,-0.00020494,-0.00008196,0.00191172,-
0.00121994,0.0003300
4,-0.00027439,-0.00010118,-0.00050746,-0.00114551,0.00114983,-
0.000039
72,-0.00006140,0.00000127,0.00180353,-0.00050615,-0.00081998,-
0.000076
90,-0.00008603,-0.00007129,0.00328366,-0.22841528,0.08188968,-
0.036466
14,0.55781208,0.02003386,-0.00823021,-
0.00050898,0.02612687,0.03524655
,-0.06513336,0.01345474,0.00396475,-
0.00081769,0.00607550,0.00285756,-
0.00611439,-0.02113281,0.00883319,-0.00437850,-
0.00541047,0.00459980,-
0.00109452,0.00030447,0.00031319,0.00019259,-0.00978437,-0.00628278,-
0
.00583179,-0.00224551,-0.00045489,-0.00097312,-
0.00311886,0.00082564,0
.00555124,-0.00015322,-0.00003083,0.00029494,0.00171845,-
0.00453830,0.
00063648,-0.00008848,-0.00025311,-0.00034095,0.00201841,0.00221675,-
0.
00243587,0.00011149,0.00005387,0.00010439,-
0.00339254,0.00104903,0.000
66776,0.00001961,-0.00013248,-0.00000192,0.01207953,0.07644197,-
0.1110
5894,-0.02210080,-0.17535556,0.25396577,0.00440170,-
0.00760621,0.00301
172,-0.05531071,0.01051928,-0.00896957,0.00189986,0.00156854,-
0.000594
51,0.00279982,0.00291053,-0.00129236,-0.00710335,-0.00164216,-
0.001335
95,0.00085510,0.00824673,-0.00137159,-0.00006693,-0.00028875,-
0.000418
81,0.00055853,-0.00297807,0.01433208,0.00079461,-0.00059634,-
0.0007378
1,-
0.00297835,0.00143960,0.00132265,0.00005983,0.00006471,0.00000917,0
.00055091,-0.00225005,0.00050322,-
0.00006046,0.00005701,0.00000574,0.0
0070766,0.00120034,-0.00115727,0.00003803,0.00003518,-0.00000638,-
0.00
124980,0.00061787,0.00038802,0.00001021,-
0.00000703,0.00005331,0.03765
726,0.04178113,-0.02650327,-0.22774048,0.06949302,-
0.02017628,0.671685
54,-0.00387135,-0.00106532,0.00120737,-
0.00256559,0.01492661,0.0002993

This journal is © The Royal Society of Chemistry 2014

7,-0.00152960,0.00026503,-0.00114594,-0.00073114,-
0.00080828,0.0000129
2,0.00001332,-0.00408801,0.00542885,-0.00128077,-0.00278547,-
0.0001424
6,-0.00002484,0.00009396,0.00014971,-0.00165034,0.00092102,-
0.00476269
,0.00014838,0.00049888,0.00060365,0.00032769,0.00126007,0.00008950,-
0.
00006377,-0.00009075,-0.00001988,-0.00032789,0.00019812,0.00027362,-
0.
00015704,0.00004164,-0.00005600,-0.00008280,-0.00024234,0.00023176,-
0.
00000673,0.00002150,0.00000853,0.00019623,-0.00014628,-0.00023538,-
0.0
0005584,0.00005850,-0.00000895,0.02018345,-
0.02125431,0.01244094,0.104
48064,-
0.17299708,0.03850460,0.01310330,0.61699970,0.00231216,0.001471
49,0.00249722,0.00929027,-0.00393242,0.00491785,-0.00006013,-
0.0010417
0,-0.00143326,-0.00030930,-0.00059461,-
0.00024102,0.00370066,0.0042205
4,0.00344573,0.00014010,-0.00179409,0.00037956,-
0.00002959,0.00002202,
0.00001298,-0.00078674,0.00058923,-
0.00214177,0.00025965,0.00018760,0.
00063021,0.00045335,-0.00007762,-
0.00005892,0.00002485,0.00004618,0.00
004722,-0.00025737,0.00004513,-0.00025727,-0.00000462,-0.00002045,-
0.0
0004753,0.00008874,-
0.00020460,0.00018716,0.00000634,0.00000404,0.0000
1621,0.00000256,-0.00006973,-0.00020089,0.00003693,-0.00002924,-
0.0000
1842,-0.01464490,0.01165911,0.00164903,-0.03724129,0.04261400,-
0.07749
413,-0.05462006,-0.23473750,0.25018534,0.00007647,-
0.00025230,0.000233
75,0.00156822,0.00118282,-0.00109883,-0.00033961,-
0.00052802,0.0003269
4,0.00011725,-0.00005775,-0.00018612,0.00052874,0.00136624,-
0.00067942
,0.00002582,0.00013544,-0.00000086,-0.00000984,-
0.00001308,0.00001375,
-0.00000145,-0.00005479,0.00008276,-0.00005585,-0.00002122,-
0.00013428
,0.00001336,0.00000609,0.00001872,-0.00002214,-
0.00000126,0.00001462,-
0.00000545,-0.00000399,-0.00001671,0.00000663,-0.00000394,-
0.00000142,
-0.00000264,0.00001816,0.00001024,0.00000055,-0.00000633,0.00000371,-
0

This journal is © The Royal Society of Chemistry 2014

.00002068,-0.00006011,0.00003267,0.00001319,-0.00001488,-0.00000684,-
0
.00418320,0.00177818,-0.00002112,0.00507248,0.02388952,-0.01175203,-
0.
06086082,-0.01590926,0.01061304,0.06045782,0.00036775,-0.00004210,-
0.0
0034517,-0.00193882,-0.00004336,-0.00110168,0.00086869,0.00047001,-
0.0
0016958,0.00006772,0.00020079,-0.00000006,-0.00104665,-
0.00064007,0.00
033193,0.00016082,0.00006082,0.00007613,0.00000473,-0.00001662,-
0.0000
4835,-0.00001518,-
0.00007165,0.00002605,0.00000616,0.00001664,0.000048
65,-0.00006981,-
0.00008564,0.00008881,0.00002648,0.00002268,0.00000025
,0.00005893,-0.00009094,-0.00001363,0.00001245,-0.00000457,-
0.00000489
,0.00004810,0.00002764,-0.00006214,0.00000885,0.00000172,-
0.00000325,-
0.00002394,0.00007368,-0.00001787,-
0.00000672,0.00000820,0.00001480,0.
00332605,0.00125449,0.00165904,-0.00192103,-0.01208717,0.00771311,-
0.0
1682481,-0.27585802,0.11830092,0.01742130,0.29105272,0.00023066,-
0.000
21779,0.00005521,0.00014198,-0.00176798,-0.00218735,-
0.00041368,0.0000
4125,0.00021147,0.00009673,-0.00006211,-
0.00009116,0.00008326,0.000300
19,-0.00002633,0.,0.00007035,-0.00007573,-
0.00000257,0.00002707,0.0000
0870,-0.00043184,0.00006875,-0.00008661,-0.00015613,-0.00004426,-
0.000
20658,-0.00001247,-
0.00002193,0.00006863,0.00000788,0.00000971,0.00001
355,0.00002892,-0.00005488,-0.00000306,0.00000203,-0.00000784,-
0.00000
631,0.00001698,0.00002610,-
0.00002625,0.00000211,0.00000156,0.00000511
,-0.00003091,-0.00002524,0.00001602,0.00001196,-
0.00000765,0.00000373,
-
0.00028289,0.00187098,0.00507757,0.00180550,0.00466296,0.00081441,0.0
0956086,0.11950101,-0.09505728,-0.01217208,-0.13145557,0.09003082,-
0.0
0334368,0.00152914,-
0.00118287,0.01000941,0.00732439,0.00256718,0.0000
3757,-0.00040076,0.00015214,-0.00219205,-
0.00177841,0.00035941,0.00593
809,-0.00095546,0.00259723,-0.00198030,-0.00470377,-0.00025232,-
0.0000

3896,0.00028862,0.00030446,0.00028992,0.00266724,-0.00669093,-
0.000314
34,-0.00008813,0.00010689,0.00112860,0.00011865,-0.00049683,-
0.0000588
6,-0.00008662,-0.00002795,-0.00032769,0.00110457,-0.00008432,-
0.000065
16,0.00000568,-0.00002607,-0.00047523,-0.00060607,0.00070579,-
0.000017
99,0.00000185,0.00001045,0.00081328,-0.00038920,-0.00032297,-
0.0000455
0,0.00003231,-0.00004413,-0.01992710,-0.01700096,0.01188129,-
0.0635327
3,0.01971463,-0.00243424,-0.31784938,-
0.10315659,0.07156127,0.00286072
,0.00130949,-0.00021075,0.73622422,-0.00337938,0.00327175,-
0.00211956,
0.01656642,0.00206509,0.00633524,0.00014028,-0.00015304,-0.00015742,-
0
.00332856,-0.00203091,0.00157086,0.00954204,-0.00172451,0.00315530,-
0.
00030438,-0.00685623,0.00016731,0.00006449,0.00015426,0.00017525,-
0.00
097307,0.00242240,-0.00805184,-
0.00004265,0.00017048,0.00048192,0.0016
2507,-0.00061447,-0.00102109,-0.00004914,-0.00005701,-0.00002087,-
0.00
054434,0.00162543,-0.00020060,0.00002729,0.00000803,0.00001304,-
0.0006
6413,-0.00113299,0.00110208,-0.00005496,-0.00003350,-
0.00003114,0.0016
8157,-0.00052014,-0.00044418,-0.00003676,0.00002067,-0.00005940,-
0.031
70604,-0.02290595,0.01311223,-0.01718476,0.04197720,-0.01204554,-
0.047
82279,-0.14867503,0.04530198,-0.02695279,-0.00622908,0.00728437,-
0.044
71738,0.56612259,0.00086804,-0.00159915,0.00148316,-
0.00847950,0.00115
484,0.00184238,-0.00005386,-0.00003432,-
0.00000598,0.00158093,0.001108
95,-0.00034380,-0.00474224,0.00060918,-
0.00237778,0.00036934,0.0037491
9,-0.00022978,-0.00006433,-0.00019694,-0.00020180,0.00140484,-
0.001130
16,0.00537434,0.00032993,-0.00010797,-0.00023136,-
0.00086524,0.0003792
2,0.00010657,0.00003771,0.00002239,0.00000552,0.00018087,-
0.00065004,0
.00013324,-0.00000323,0.00003680,0.00003487,0.00026600,0.00049804,-
0.0
0048250,0.00000902,0.00000830,-0.00000915,-
0.00069009,0.00028575,0.000

24867,-0.00000984,0.00000748,0.00002876,0.01570196,0.00939501,-
0.01350
578,0.01615571,-0.02016450,0.01236825,0.04509008,0.05240626,-
0.0884773
3,0.01322048,0.00481900,-0.00004571,-0.03028264,-
0.21064636,0.23857319
,-0.00032803,-0.00031922,-0.00005643,-0.00041576,0.00128588,-
0.0000505
1,-0.00001139,-0.00003993,-0.00000771,0.00001507,-
0.00001957,0.0000139
0,0.00010947,-0.00001606,-0.00006100,-0.00004372,-0.00003965,-
0.000019
34,-0.00000493,0.00001582,0.00000946,-0.00012233,-0.00002194,-
0.000037
77,-0.00002301,0.00002574,0.00002254,-0.00003857,0.00013674,-
0.0000007
4,-0.00000273,-0.00001313,-0.00000894,-0.00001633,-
0.00000588,0.000052
38,-0.00001933,0.00000687,0.00000252,-0.00000906,-
0.00000066,0.0000128
2,-0.00000881,0.00000458,-0.00000082,0.00001339,-
0.00000753,0.00000356
,-0.00000416,0.00000821,-0.00000546,-0.00007374,-
0.00066522,0.00031459
,-0.00304592,-0.00331924,0.00208163,-0.01887764,0.01671407,-
0.00634281
,0.00099389,-0.00038958,-0.00025200,-0.25334525,0.12279495,-
0.04204398
,0.26708875,-0.00016647,-0.00009015,-0.00017604,-
0.00032674,0.00050300
,0.00008893,0.00004077,-
0.00000762,0.00003451,0.00002964,0.00001778,0.
00005830,-0.00003346,-0.00012891,-0.00033568,0.00000780,-
0.00002282,0.
00001206,-0.00000914,-0.00000571,-0.00000710,0.00005363,0.00001201,-
0.
00002607,-0.00002225,-0.00000205,-0.00001467,-0.00002932,0.00000287,-
0
.00000463,-0.00000155,0.00000078,-
0.00000454,0.00002724,0.00000558,0.0
0001278,0.00000330,0.00000280,0.00000252,-0.00001274,0.00001587,-
0.000
01374,0.00000434,-0.00000122,-0.00000236,0.00000483,0.00000456,-
0.0000
0843,-0.00000647,0.00000846,0.00000497,-0.00088061,-
0.00062173,0.00014
217,-0.00237123,0.00111631,0.00336052,-0.01095918,0.01039368,-
0.002429
10,0.00016336,-0.00016447,-0.00213386,0.12281118,-
0.13274058,0.0371033
8,-0.13248018,0.13511903,0.00005738,0.00005063,-
0.00037278,0.00005139,

-
0.00049094,0.00013786,0.00006691,0.00002777,0.00011506,0.00003069,0.0
0010604,0.00003096,-0.00042253,-0.00024404,-
0.00067212,0.00002362,0.00
024101,0.00001104,-0.00000127,0.00001791,0.00001552,-0.00003597,-
0.000
13115,0.00025835,-0.00004248,-0.00002807,-0.00001852,-0.00003882,-
0.00
011930,-0.00004084,-0.00000187,0.00000313,-
0.00000262,0.00006327,0.000
00352,-0.00000938,0.00001675,-0.00000164,0.00001479,-
0.00001671,0.0000
4943,-0.00004463,0.00000030,-0.00000146,-0.00000110,-
0.00003279,0.0000
1512,0.00005329,0.00000390,0.00000010,0.00000120,0.00051660,-
0.0005049
9,-0.00052418,0.00233574,0.00394522,0.00596978,0.00789103,-
0.00428751,
0.00493443,-0.00064064,-0.00211845,-0.00335839,-
0.04266643,0.03693563,
-0.05131381,0.04483730,-0.04313772,0.04281089,-
0.00161576,0.00115055,-
0.00131930,0.00518047,0.00204273,0.00155254,0.00001982,-0.00006945,-
0.
00008353,-0.00329668,-0.00081320,0.00058746,0.00666105,-
0.00473670,0.0
0571113,-0.00012709,-0.00458087,0.00003535,-0.00018451,0.00007155,-
0.0
0004194,-0.00118705,0.00140683,-0.00393798,-
0.00010494,0.00011102,0.00
030110,0.00051799,-0.00012298,-0.00041866,-0.00004459,-
0.00004591,0.00
000308,-0.00031049,0.00077760,-0.00005968,-
0.00000595,0.00001528,0.000
01863,-0.00042757,-0.00060146,0.00073921,-0.00007991,-0.00002458,-
0.00
000803,0.00109432,-0.00057853,-0.00005135,-0.00005874,0.00004352,-
0.00
008058,-0.05982469,-0.00111448,0.00672419,-0.01436263,0.01777836,-
0.00
603263,0.02415823,-0.03011799,0.01234984,-0.00498037,-
0.00208698,0.002
02763,-0.12843464,-0.03692718,0.02357540,0.00586391,0.02505176,-
0.0124
8181,0.73941882,0.00327854,-0.00275912,0.00157525,-0.01137459,-
0.00394
349,-0.00355178,-0.00002509,0.00033168,-
0.00012270,0.00391428,0.003762
08,-0.00155088,-0.01804562,0.00136402,-
0.00138040,0.00275634,0.0080353
5,0.00145439,0.00019622,-0.00029842,-0.00039646,-0.00032870,-
0.0035917

5,0.00797249,-0.00003310,-0.00003761,-0.00037442,-
0.00148463,0.0002204
2,0.00066946,0.00003578,0.00005925,0.00002267,0.00047109,-
0.00163151,0
.00028721,0.00003329,-0.00000145,0.00002826,0.00074011,0.00118709,-
0.0
0127143,0.00000385,0.00001348,0.00004291,-
0.00215095,0.00050076,0.0008
8729,0.00005566,-0.00000342,0.00008061,0.03544247,0.03475048,-
0.021564
70,0.03027756,-0.03343433,0.00845523,-0.06808825,-
0.01195516,0.0178907
8,-0.00091938,0.00241685,0.00248405,0.02048865,-
0.26060674,0.09682030,
-0.00292467,-0.00996701,0.00648081,-0.00485390,0.56085352,-
0.00158849,
0.00160221,-0.00061408,0.00546836,0.00143597,0.00098485,-0.00006798,-
0
.00013975,-0.00005267,-0.00261048,-
0.00138531,0.00095688,0.00882664,0.
00206168,0.00512858,-0.00054416,-0.00315000,-
0.00020773,0.00011894,0.0
0013001,0.00017329,0.00034472,0.00149937,-0.00368033,-
0.00002797,0.000
03212,0.00002212,0.00085802,-0.00011555,-0.00025584,-0.00003500,-
0.000
03517,-0.00000628,-0.00028009,0.00088498,-0.00014948,-0.00003473,-
0.00
001270,-0.00003574,-0.00047152,-
0.00068250,0.00073700,0.00001123,0.000
00371,0.00003703,0.00096973,-0.00056543,-0.00066001,-0.00000786,-
0.000
02579,-0.00004701,-0.01029410,-0.01360017,0.01576116,-
0.01524126,0.012
70212,-0.00985856,0.03336495,0.01160710,-
0.00228636,0.00161338,0.00274
646,0.00621580,-0.00509905,0.10003532,-
0.11114814,0.00112911,0.0042642
3,0.00077520,-0.04651008,-
0.21095296,0.23928553,0.00001360,0.00001903,
-0.00002920,0.00007250,-0.00007888,-0.00002612,-0.00002016,-
0.00001539
,0.00001958,-0.00029548,0.00019667,-0.00027406,-0.00044782,-
0.00073956
,0.00088572,-0.00017371,0.00001495,-0.00008010,-
0.00001586,0.00001219,
0.00003476,-0.00000752,0.00000559,0.00000713,-0.00000673,-
0.00000455,0
.00000999,0.00001952,0.00001208,-0.00000359,-0.00000194,-
0.00000728,0.
00000067,-0.00000793,0.00001825,0.00000307,-0.00000959,-
0.00000217,0.0

0000264,-0.00002248,0.00004269,0.00002571,-0.00001932,-
0.00000037,0.00
000573,-0.00003383,-0.00007533,0.00010390,-0.00000459,0.00000545,-
0.00
001388,-0.00200741,0.00382963,-0.00148624,0.00018415,0.00057289,-
0.000
36732,0.00156984,0.00017889,0.00021635,-0.00000425,0.00015484,-
0.00004
954,0.00236515,0.00113678,-0.00056556,0.00073239,-0.00045988,-
0.000100
21,-0.28405835,-0.09144703,0.06479578,0.30042140,0.00002548,-
0.0000832
8,0.00006166,-0.00041355,-0.00011515,-
0.00037333,0.00005567,0.00003913
,-0.00001716,0.00019191,-0.00028354,-
0.00007725,0.00031909,0.00056971,
-0.00047010,-0.00001388,0.00021582,-0.00000790,-0.00001666,-
0.00000096
,-0.00001520,-0.00001390,-
0.00009853,0.00024944,0.00001114,0.00000384,
0.00001835,-0.00003319,0.00003211,0.00003111,0.00000762,0.00000232,-
0.
00000212,-0.00000680,-0.00004933,0.00000770,-0.00000170,0.00000108,-
0.
00000061,0.00004841,-0.00000826,-
0.00001586,0.00001502,0.00000934,0.00
000323,-0.00002723,0.00005886,-0.00011144,-0.00000041,-
0.00000189,0.00
000423,0.00341662,-0.00008737,0.00401911,0.00095322,-0.00062037,-
0.000
25584,0.00100272,-0.00359809,0.00459364,-0.00133504,-
0.00039172,0.0004
0820,-0.02675657,-0.00561811,0.00631213,0.00022727,0.00024497,-
0.00169
792,-0.09189557,-
0.09352028,0.03534950,0.09801505,0.09351483,0.0000426
6,-0.00002503,0.00013762,-0.00031503,-0.00043601,-0.00064577,-
0.000035
37,0.00000943,0.00002842,-0.00009414,-0.00029334,-0.00038417,-
0.000412
55,0.00010760,0.00039743,0.00008019,0.00015521,0.00001355,-
0.00003490,
-0.00001833,-0.00001749,-0.00003658,-0.00006711,0.00016284,-
0.00000924
,-0.00000559,-0.00001123,-
0.00001598,0.00000678,0.00002630,0.00000018,
0.00000211,0.00000668,-0.00001629,-0.00005349,0.00000422,0.00000328,-
0
.00000172,-
0.00000288,0.00006440,0.00001523,0.00000385,0.00001201,0.00
000670,0.00000738,-0.00007090,0.00003069,-0.00005477,-0.00000122,-
0.00

000507,-0.00000169,-0.00043823,0.00336162,0.00619300,-
0.00020006,0.000
34368,-0.00081175,-
0.00043643,0.00469135,0.00365216,0.00071951,0.00026
906,0.00001882,0.01346337,0.00447250,-0.00046447,-0.00046588,-
0.001686
74,-0.00237012,0.06479404,0.03520788,-0.05872190,-0.07004123,-
0.041282
34,0.05115071,0.00298595,-0.00319014,0.00211444,-0.00873481,-
0.0013651
8,-0.00377276,0.00058573,0.00063890,-
0.00004861,0.00686319,0.00637732,
-0.00460403,-0.05351285,-0.00060198,-
0.00027868,0.00197000,0.01059890,
0.00247262,0.00046675,-0.00035260,-0.00083508,-0.00023032,-
0.00436088,
0.00781094,0.00001135,-0.00013863,-0.00035177,-
0.00126028,0.00015419,0
.00071700,0.00002832,0.00004624,0.00000837,0.00054692,-
0.00191231,0.00
034401,0.00003204,-0.00002592,0.00002744,0.00105088,0.00186976,-
0.0017
9792,-0.00001315,0.00000002,0.00005955,-
0.00374896,0.00074903,0.001781
18,0.00009520,-0.00006527,0.00007966,-0.24198469,-
0.04778132,0.0394573
7,0.02827760,-0.05235679,0.02067480,-
0.05751267,0.00476803,0.00466475,
-0.00107695,0.00021958,-0.00016516,0.03727909,0.05988904,-
0.03124616,0
.00131955,-0.00172594,0.00110263,-0.28996500,0.07719460,-0.02070053,-
0
.01930174,0.01664537,-0.00634607,0.65703190,-0.00004597,0.00028690,-
0.
00035868,0.00334780,-0.00374087,0.00510434,-0.00148170,-
0.00057647,0.0
0006553,0.00326034,-0.00153325,0.00298716,0.01595846,0.01103738,-
0.007
62326,-0.00030586,-
0.00076962,0.00010936,0.00000847,0.00020986,0.00005
592,0.00098369,0.00080506,-0.00077906,0.00000548,-
0.00000752,0.0000764
9,0.00000527,-0.00002364,-0.00002058,0.00005660,0.00002679,-
0.00006116
,0.00003525,0.00018723,-0.00004451,0.00000271,0.00000896,-
0.00000510,-
0.00008965,-0.00044333,-0.00008436,0.00010125,0.00002540,-
0.00003830,0
.00065340,0.00034189,-0.00096604,0.00008544,-0.00001115,0.00007446,-
0.
07751559,-0.13198828,0.04716635,-0.03167071,-
0.01023157,0.01057871,0.0

0839766,-0.00248234,-0.00199927,0.00017275,0.00038647,-
0.00029533,0.01
974732,-0.03072253,0.01753534,-0.00077219,-
0.00318111,0.00457484,0.132
19800,-0.17961819,0.04842951,-0.01134701,0.00975796,-0.00270595,-
0.041
10919,0.62159006,-0.00085888,0.00047746,-
0.00089362,0.00249637,0.00514
264,0.00341931,0.00064336,0.00028682,0.00010538,-
0.00182178,0.00289915
,0.00183932,0.00145007,-0.00594696,0.00802642,-0.00172452,-
0.00286944,
-0.00083840,0.00016031,0.00046717,0.00066786,-0.00037666,0.00112094,-
0
.00266632,-0.00007781,0.00001501,0.00009735,0.00016118,-0.00017220,-
0.
00024065,-0.00003567,-0.00002181,0.00001216,-0.00001426,0.00042453,-
0.
00009384,0.00000666,-0.00000022,0.00003141,-0.00050346,-
0.00005792,0.0
0020015,-0.00014177,-0.00006672,-0.00002518,0.00050144,-
0.00069371,0.0
0085668,0.00001878,0.00004171,0.00001298,0.05204689,0.04400619,-
0.0926
9802,0.01217645,0.01106311,0.00014246,0.00231417,-0.00156667,-
0.004065
09,-0.00003070,-0.00048606,-0.00047884,-
0.01323039,0.01155202,0.002381
49,0.00076631,0.00461625,0.00359778,-0.04877740,0.05554610,-
0.08380905
,0.00737902,-0.00450661,0.00517346,-0.02373966,-
0.24210992,0.25654985,
0.00015822,-0.00008976,-0.00015004,0.00047377,-
0.00143562,0.00079579,-
0.00047204,-
0.00017762,0.00004220,0.00017132,0.00032243,0.00004492,0.0
0111666,-0.00102202,-0.00017511,-0.00004279,0.00009636,-0.00000696,-
0.
00002868,-0.00006613,-0.00006569,-0.00001340,-0.00004716,0.00016618,-
0
.00000976,0.00003074,0.00001070,-0.00002807,0.00006324,-
0.00004078,0.0
0001786,0.00000889,-0.00001842,-0.00000232,0.00000495,0.00003183,-
0.00
000055,0.00001065,-0.00000246,-0.00003166,0.00001205,-
0.00001594,0.000
00139,0.00000157,-0.00000240,0.00003287,-0.00004357,-0.00000095,-
0.000
04600,0.00004994,0.00001405,0.00282890,-0.02518667,0.01264845,-
0.00499
901,-0.00058301,0.00103907,-
0.00114878,0.00004292,0.00003716,0.0001760

0,-0.00008081,-0.00008231,-0.00417834,0.00252578,-
0.00026855,0.0001477
1,0.00124532,-0.00058106,0.00619164,0.02505779,-
0.01265818,0.00098960,
-0.00047553,-0.00024802,-0.06130656,-
0.02126613,0.01351869,0.06271961,
0.00000808,-0.00011334,-0.00012487,0.00031360,-
0.00041309,0.00031632,-
0.00014675,-0.00004347,0.00006226,0.00003877,0.00012847,-
0.00016128,0.
00060350,-0.00114855,-0.00051256,-0.00031271,-0.00006875,-
0.00005500,-
0.00007566,-0.00007578,-0.00005322,-0.00003827,-
0.00003745,0.00004283,
-0.00000353,0.00000498,0.00003135,-0.00000027,0.00003846,-
0.00001668,0
.00000671,0.00000146,-0.00000734,-0.00000582,0.00000798,0.00001081,-
0.
00000365,0.00000659,0.00000317,-0.00002415,0.00002805,-0.00000932,-
0.0
0000814,0.00000013,-0.00000180,0.00004633,-0.00001250,0.00003524,-
0.00
002076,0.00004052,0.00000623,-0.00000203,-0.00602513,0.00459005,-
0.001
42590,0.00221545,0.00189227,-0.00009895,0.00027805,-0.00049196,-
0.0000
5969,-0.00030102,-0.00043251,0.00344584,0.00172861,0.00280198,-
0.00021
502,-0.00057055,0.00039678,-0.00304424,-
0.01123465,0.00754531,0.000008
79,-0.00008525,-0.00225050,-0.02157455,-
0.27903681,0.12155460,0.019543
20,0.29441143,0.00004007,-0.00013331,0.00001744,-
0.00060927,0.00039363
,-0.00015516,0.00019170,0.00005418,0.00016479,0.00050278,-
0.00009633,-
0.00021328,-0.00137156,-0.00010809,-0.00247074,-
0.00018601,0.00000961,
-0.00003445,-0.00005405,-0.00005676,-0.00005026,0.00007758,-
0.00003233
,0.00010652,0.00001247,-0.00002774,0.00000171,-0.00004842,-
0.00001208,
0.00003348,0.00000666,0.00000707,0.00000709,0.00003846,-0.00008846,-
0.
00000743,0.00000778,-0.00000231,-0.00000116,0.00008897,0.00006059,-
0.0
0009643,0.00001321,-0.00000129,-0.00000934,-
0.00005623,0.00014190,0.00
005767,0.00001631,-0.00001081,0.00000882,0.00184672,0.00723376,-
0.0008
6273,0.00231301,0.00178814,0.00433194,-0.00026021,-0.00057675,-
0.00034

This journal is © The Royal Society of Chemistry 2014

052,-0.00011825,-0.00040308,-0.00092729,-
0.00077030,0.00307556,0.00642
302,0.00012537,0.00028644,-
0.00000132,0.00164592,0.00521278,0.00120654
,-0.00044259,-0.00224445,-0.00355293,0.01188948,0.12079154,-
0.09613346
,-0.01263127,-0.13542760,0.09282208,0.00034794,0.00026997,-
0.00014375,
-0.00662954,-0.00724793,-
0.02061319,0.00089166,0.00055506,0.00160650,0
.00157761,-0.00008333,-0.00022626,0.00377793,0.00207520,0.00498516,-
0.
01650482,-0.02601907,0.00973459,-0.00186203,0.00413755,-0.00048623,-
0.
18530780,-0.01367188,0.02547405,-0.01028143,-0.00633463,-
0.00277293,0.
00040935,0.00149729,-0.00036757,0.00026552,-0.00024096,0.00066605,-
0.0
0084301,-0.00033211,-0.00022230,-0.00016256,0.00015039,0.00033805,-
0.0
0066280,0.00131691,-0.00030696,-0.00008501,0.00008598,0.00012005,-
0.00
103094,0.00001025,0.00099986,-0.00001450,0.00029035,0.00007554,-
0.0028
3968,0.00261238,0.00050330,-0.00051433,-
0.00032342,0.00083612,0.000935
68,0.00074870,-0.00001966,-0.00008033,0.00004369,0.00013280,-
0.0007821
0,-0.00034493,-0.00018426,0.00018596,-
0.00006098,0.00000158,0.00020526
,0.00128145,-0.00067124,0.00009974,0.00006463,0.00000741,0.00145294,-
0
.00061571,-0.00005991,0.00013445,0.00015778,-0.00006645,0.58523728,-
0.
00231422,-0.00033268,-0.00068642,-0.00808617,-0.00326181,-
0.00912232,0
.00197060,0.00016623,0.00296185,-0.00037040,-0.00033457,0.00081141,-
0.
00338198,-0.00424916,-0.00407667,-0.01817133,-
0.00939346,0.01058679,0.
00352278,-0.00366990,0.00272352,-0.00381742,-
0.08950872,0.00968356,0.0
2413839,0.00892484,-0.00450952,0.00058094,0.00157821,-
0.00165380,0.000
16399,-0.00039549,0.00142949,-0.00043149,0.00012392,0.00000418,-
0.0001
8295,0.00011022,0.00012655,0.00016937,-0.00039523,0.00030083,-
0.000071
41,-0.00008723,-0.00000502,0.00053807,-0.00112709,0.00035489,-
0.000068
13,-0.00021882,-0.00017071,0.00140946,-
0.00170885,0.00099978,0.0033438

This journal is © The Royal Society of Chemistry 2014

4,-0.00045374,-0.00017118,-
0.00114417,0.00126607,0.00014466,0.00008392
,-0.00015936,0.00006623,0.00097476,0.00049597,-
0.00032668,0.00008938,-
0.00002955,-0.00004214,0.00020458,-0.00111255,0.00043925,0.00008764,-
0
.00002116,-0.00003140,-0.00076847,-0.00010767,0.00058210,-
0.00013235,-
0.00001148,0.00000669,0.24621969,0.75975954,-0.00103979,-0.00228554,-
0
.00172608,-0.01114955,-0.00440177,-0.00305276,-
0.00102863,0.00035184,-
0.00114980,-0.00154665,0.00015887,0.00142052,-0.00090301,0.00066155,-
0
.00107698,0.01595568,0.01824966,-0.01006877,-
0.00118224,0.00641907,0.0
0104955,0.00042419,-0.00565385,-0.06031247,0.00146710,0.00280446,-
0.00
126369,0.00064399,-0.00141738,-0.00087949,-0.00007345,0.00023224,-
0.00
103827,0.00011335,0.00065665,-0.00005493,-0.00000247,-0.00002739,-
0.00
012520,-0.00047203,-
0.00063033,0.00050859,0.00002711,0.00011632,0.0000
3054,0.00080738,0.00034131,-
0.00100474,0.00001408,0.00019595,0.0000999
7,0.00084365,-0.00143076,-0.00106483,-0.00081382,-0.00018301,-
0.002443
43,-0.00059654,-0.00041036,-0.00020914,-0.00010445,0.00008274,-
0.00016
537,0.00041128,0.00031947,0.00002049,-0.00003957,0.00004221,-
0.0000154
3,-0.00013441,-0.00046137,0.00037582,-
0.00002404,0.00000113,0.00000569
,-0.00053801,0.00046547,-0.00031057,0.00005382,-0.00001595,-
0.00002054
,-0.12051698,-0.27546594,0.34299574,0.00340647,-0.00101872,-
0.00016384
,0.00531345,0.00537950,0.01150183,0.00008520,-
0.00025029,0.00015202,0.
00066265,-0.00034442,0.00011727,-0.00521499,-0.01608906,-0.01566583,-
0
.20187654,0.03798505,-0.00140501,-0.01182528,0.00272185,-0.00835448,-
0
.01227080,0.02312400,-0.02862344,-0.00211213,-0.00201224,0.00404727,-
0
.00185460,0.00133108,0.00080208,0.00004424,-0.00019437,0.00052624,-
0.0
0107764,-0.00135636,0.00120394,-0.00009872,0.00005147,0.00019733,-
0.00
068013,-0.00030024,-0.00038037,-
0.00018128,0.00022970,0.00031086,0.000

24271,-0.00059074,0.00095617,0.00029817,0.00050287,0.00018588,-
0.00086
913,0.00162526,0.00122427,-0.00381535,-
0.00063895,0.00264949,0.0017370
8,0.00027165,-0.00045970,0.00009125,-
0.00023224,0.00013214,0.00035362,
-0.00141538,0.00073216,0.00010546,-0.00007033,0.00001664,-
0.00074086,-
0.00029636,-0.00024972,0.00024176,0.00002778,-0.00005756,0.00048230,-
0
.00045452,0.00067229,-0.00002763,0.00018819,0.00007380,0.06198392,-
0.0
3785710,0.01634672,0.54863483,-0.00206363,0.00135797,0.00086128,-
0.000
38947,-0.00255149,-0.00064854,0.00027155,0.00007594,0.00036220,-
0.0000
3009,-0.00026722,-0.00200566,-
0.00175474,0.00681389,0.00165306,0.01556
053,-0.07428461,0.00808144,-0.01030022,0.00329641,-
0.00126251,0.023196
00,-0.02535637,0.01703389,-0.00262403,-
0.00380157,0.00577337,0.0010634
2,-0.00127434,-0.00031523,0.00009806,-0.00005823,0.00039482,-
0.0005436
5,0.00103650,-0.00045377,0.00003980,-
0.00001920,0.00012188,0.00011797,
-0.00002205,0.00055027,0.00007360,-0.00016440,-
0.00016792,0.00042750,0
.00020257,-0.00100804,-0.00016353,-0.00105888,-0.00050773,-
0.00175094,
-0.00126661,-0.00112331,0.00057210,-0.00057874,-0.00177821,-
0.00039208
,-0.00069275,0.00004855,0.00007116,0.00001304,-0.00000315,-
0.00024455,
0.00025662,0.00005114,-0.00005767,0.00001098,0.00002454,-
0.00001787,0.
00018891,0.00007894,-0.00010266,-
0.00002570,0.00002773,0.00035621,0.00
021734,-0.00072510,-0.00026835,-0.00024081,0.00005925,0.01909910,-
0.07
574036,0.03674105,-0.22205774,0.67292090,-0.00189565,0.00133382,-
0.000
33311,-0.00254019,-0.00141193,-0.00617784,-0.00002796,0.00009153,-
0.00
023606,-0.00110583,-0.00015359,-0.00106361,-0.00805812,-0.00714785,-
0.
00630608,-0.00706092,0.02534750,-0.07912457,0.01840788,-
0.00976020,0.0
0480113,-
0.01172241,0.00674029,0.00210915,0.00282464,0.00218891,0.0014
1755,0.00115424,0.00027771,-0.00048114,-0.00009244,-0.00001730,-
0.0002

5019,-0.00000324,0.00074212,-0.00017747,-0.00004934,0.00000373,-
0.0000
2634,-0.00041685,-0.00043682,0.00035954,-
0.00012813,0.00003725,0.00010
260,0.00063941,-0.00140961,-
0.00058154,0.00005424,0.00050530,0.0002403
4,0.00188815,0.00023137,0.00004064,0.00116756,0.00112369,-
0.00170525,-
0.00041892,0.00027016,0.00006360,-0.00005310,0.00002707,-
0.00001704,0.
00011346,0.00074953,-0.00035438,0.00005989,-0.00000507,-
0.00001504,0.0
0071286,-0.00048063,0.00021372,0.00006188,-0.00002594,-0.00001789,-
0.0
0105692,-0.00044267,0.00036124,0.00011950,0.00010445,-0.00008266,-
0.01
749912,0.04493923,-0.03192235,0.14516590,-
0.32614139,0.42338638,0.0003
8164,0.00006060,0.00014811,0.00053442,0.00127407,0.00320801,-
0.0001029
6,-0.00011711,-0.00009099,-0.00005753,-
0.00019588,0.00015395,0.0006084
2,0.00255573,0.00339563,-0.04765991,-0.01889962,0.01710476,-
0.00531467
,0.00251275,-0.00342185,-0.04163259,0.02618882,-0.00806979,-
0.00577589
,-0.00363121,0.00002667,-0.00007181,-0.00002704,-0.00016943,-
0.0000740
6,0.00003898,-0.00017348,0.00077000,-0.00013157,-
0.00015059,0.00004387
,-0.00003782,-0.00011252,0.00062784,0.00002014,-
0.00019957,0.00004290,
-0.00006306,-0.00009227,-0.00009165,0.00010646,-0.00005184,-
0.00007840
,-0.00006576,-0.00001751,-0.00144443,0.00019306,-0.00125274,-
0.0020072
7,-0.00097434,-0.00043411,0.00095384,-0.00072363,-
0.00043282,0.0000104
1,0.00008592,0.00005034,-0.00057541,-0.00058206,0.00034200,-
0.00004790
,0.00004498,0.00005592,-0.00038015,0.00079761,-0.00030592,-
0.00006125,
0.00001993,0.00006230,0.00098479,0.00002944,-0.00059774,0.00000648,-
0.
00002469,0.00005678,-0.18249834,0.03201308,-0.01281220,-0.17727165,-
0.
00916277,0.01313209,0.38951550,-0.00016025,0.00003941,-0.00063828,-
0.0
0113080,-0.00296856,-0.00596991,-0.00031521,0.00035791,-0.00036984,-
0.
00071088,-0.00014852,0.00045677,0.00330569,0.00287374,0.00447282,-
0.02

This journal is © The Royal Society of Chemistry 2014

146598,-0.00433977,0.00824472,-0.00149033,0.00368896,-
0.00040973,0.022
40464,-0.00091534,0.01432873,0.00127884,0.00186549,-
0.00040862,0.00033
640,-0.00050072,-0.00006594,-0.00006178,0.00014883,-
0.00067735,0.00002
585,0.00024951,-0.00020784,0.00003530,-0.00001649,-0.00008109,-
0.00037
217,0.00022991,0.00006440,0.00000782,0.00007324,0.00004346,-
0.00003898
,0.00049415,-0.00003737,0.00000625,0.00035630,0.00019629,-
0.00056741,0
.00105929,0.00009354,0.00044724,0.00063978,0.00010363,-
0.00009536,0.00
018706,0.00027871,-0.00012720,0.00013441,-0.00009795,-
0.00053558,0.000
21278,-0.00018498,0.00001177,0.00000641,-
0.00001708,0.00027202,0.00067
806,-0.00032136,-0.00003081,0.00003267,0.00002762,0.00049373,-
0.000094
19,-0.00035133,0.00019968,0.00010694,-0.00002840,0.04236418,-
0.0852337
5,0.01190988,-0.01506625,-0.05723693,0.00324110,-
0.02066619,0.28476091

,0.00003017,0.00039987,0.00002096,0.00369879,0.00134986,0.00342196,0.0
0005754,-0.00018084,0.00016830,-0.00042299,-0.00072120,-
0.00019719,0.0
0049435,-0.00214781,-
0.00361397,0.01696531,0.00619219,0.01328783,0.000
32889,0.00049799,0.00177093,-0.01104485,0.01651032,0.00327102,-
0.00198
001,-0.00178775,0.00242334,-0.00027945,-0.00013740,-
0.00008594,0.00006
521,-0.00005970,0.00035050,-
0.00062499,0.00005578,0.00016817,0.0000075
0,0.00002582,0.00008951,-0.00020499,-
0.00005418,0.00012115,0.00000338,
-0.00003966,-0.00001266,0.00013463,0.00009341,0.00011014,0.00001695,-
0
.00024632,-0.00013281,-0.00007407,0.00020485,0.00096717,-
0.00061156,0.
00002665,0.00166501,0.00036006,-0.00004953,-0.00016333,0.00008791,-
0.0
0008428,0.00009269,0.00011213,-0.00048333,0.00016370,0.00000074,-
0.000
01119,0.00001780,-0.00033540,-0.00007059,-0.00004863,0.00002363,-
0.000
00448,-0.00001022,0.00008239,0.00005939,0.00027401,-0.00010678,-
0.0000
4292,0.00003723,-0.01821853,0.00937168,-
0.06123608,0.01533061,0.004929

87,-0.06138606,-0.01124449,-0.13652989,0.13237950,-
0.00095694,0.000586
82,0.00011252,-0.00137802,-0.00077105,-0.00240978,-0.00005862,-
0.00007
363,-0.00018453,-0.00062778,-
0.00008338,0.00016986,0.00023193,0.003504
82,0.00319248,-0.01321874,0.03750935,-0.03032805,0.00180990,-
0.0003639
8,0.00099280,-0.00632186,-
0.00111785,0.00447691,0.00082274,0.00145393,
-0.00213427,0.00040542,-0.00048086,-0.00009670,-
0.00000493,0.00004360,
-0.00006668,0.00026882,0.00033974,-0.00031031,0.00004179,-
0.00002079,-
0.00007014,0.00030515,0.00003952,0.00012162,0.00008362,-0.00011191,-
0.
00016513,0.00015914,0.00031672,-0.00007612,-0.00020130,-0.00034226,-
0.
00015461,0.00048626,-0.00054703,-0.00023998,0.00132531,0.00023901,-
0.0
0068442,-0.00067825,-0.00014618,0.00010999,-0.00000003,0.00006107,-
0.0
0002120,0.00002421,0.00049208,-0.00023928,-0.00005043,0.00002756,-
0.00
001579,0.00025145,-0.00003550,0.00017330,-0.00008725,-
0.00001836,0.000
02219,-0.00027179,0.00019021,-0.00023376,-0.00000036,-0.00007336,-
0.00
003094,-0.00962896,0.00326291,-0.00057630,-0.19801394,0.19359936,-
0.13
552187,0.03434025,-0.01990934,0.01322500,0.19051735,0.00209522,-
0.0015
4834,-0.00074553,0.00174235,0.00177608,0.00322835,-
0.00006449,0.000073
79,0.00002176,0.00059184,0.00028996,-0.00056213,-0.00089634,-
0.0074982
6,-0.00217109,0.02831950,-0.01312777,0.02694897,0.00000431,-
0.00100441
,-0.00206737,0.00377616,0.00528711,-0.00584197,0.00074974,-
0.00008952,
0.00041399,-0.00101049,0.00087304,0.00027858,-0.00003281,0.00001792,-
0
.00018636,0.00024628,-0.00087898,0.00038089,-0.00002960,0.00002917,-
0.
00002358,-0.00015548,0.00023715,-0.00047203,-
0.00007742,0.00012371,0.0
0016414,-0.00062466,-
0.00051734,0.00035967,0.00009263,0.00077251,0.000
36609,-0.00027013,0.00175359,0.00045810,-0.00273438,-
0.00030107,0.0009
5949,0.00142625,0.00016266,-0.00029831,-0.00004861,0.00000064,-
0.00000

152,-0.00040051,-0.00080928,0.00040539,0.00004819,-
0.00001205,0.000006
56,-0.00030828,0.00046995,-0.00037835,0.00009071,0.00003659,-
0.0000080
3,0.00049356,-0.00035992,0.00020562,0.00021148,0.00019671,-
0.00003351,
-0.01925542,0.01620600,-0.00317398,0.19644735,-
0.45020120,0.26677378,-
0.00080930,-0.06532974,0.05133585,-0.21267797,0.51874279,-
0.00012797,0
.00042484,0.00004408,-0.00055272,-0.00039089,-0.00017950,0.00005723,-
0
.00002727,0.00008935,-0.00082414,-
0.00083270,0.00018989,0.00170641,0.0
0400055,0.00208674,-0.01915485,0.01793429,-0.00009711,-
0.00195467,0.00
110172,0.00006095,-0.00384814,0.00113473,0.00392367,-
0.00037270,0.0003
9412,-0.00168018,-0.00022173,-
0.00014660,0.00006495,0.00001504,0.00002
077,0.00010207,-0.00001879,-
0.00022950,0.00001073,0.00003928,0.0000046
9,-0.00001569,0.00016933,0.00020463,-0.00009660,0.00008207,-
0.00002535
,-0.00003611,-0.00007340,0.00043398,0.00028439,-0.00005912,-
0.00009411
,-0.00008308,-0.00030700,-0.00052445,-0.00034567,0.00091782,-
0.0001336
7,0.00000905,-0.00057736,-
0.00009469,0.00014839,0.00002532,0.00001824,
-0.00000403,0.00009476,0.00023272,-0.00011490,-
0.00005105,0.00001105,-
0.00002469,-0.00001232,0.00003153,0.00013953,-0.00008498,-
0.00001804,0
.00000161,0.00004011,0.00026596,-0.00020545,-0.00005137,-0.00011527,-
0
.00003376,0.01317340,-0.00824354,0.00765224,-0.13426767,0.26411923,-
0.
25311837,-0.00119210,0.05419183,-0.02200829,0.15007112,-
0.33849766,0.2
6785004,-0.00091566,0.00058743,0.00031887,-
0.00014533,0.00008887,0.004
29907,-0.00011490,0.00005021,0.00004385,-0.00069359,-
0.00026174,0.0004
6335,-0.00112460,-0.00001954,-0.00073020,-0.00754839,0.00288712,-
0.000
12913,0.00077001,-0.00259659,0.00066237,-0.01576753,-
0.04242825,0.0166
4285,0.00159406,0.00073738,0.00023222,0.00027891,-
0.00052608,0.0003609
5,-0.00024192,0.00014590,-0.00047367,0.00038697,0.00018713,-
0.00000376

,0.00009030,-0.00010010,-0.00019316,0.00017432,-
0.00031693,0.00006809,
0.00003525,-0.00003680,-0.00006361,0.00024373,0.00022439,-
0.00032923,-
0.00000504,-0.00003892,0.00001202,0.00125862,-0.00095905,-
0.00008696,0
.00082327,0.00004215,-0.00072598,-0.00058334,-
0.00023886,0.00005890,0.
00002420,0.00001719,-0.00004232,0.00033956,0.00034812,-0.00006675,-
0.0
0007579,0.00003325,-0.00000802,0.00009416,-0.00053598,0.00028929,-
0.00
005743,-0.00003104,0.00000135,-0.00066980,0.00025304,-0.00000651,-
0.00
001501,-0.00004531,0.00003008,-0.23781215,-0.24209627,0.11627143,-
0.00
709043,-0.00029013,0.00133648,0.03644662,0.01159354,-
0.00589896,0.0014
9772,0.00274052,-0.00174469,0.22886926,-0.00038243,0.00072686,-
0.00042
216,0.00193898,0.00024348,0.00502219,-0.00073802,-0.00001218,-
0.001337
36,-0.00064337,-0.00025787,0.00040143,-
0.00006515,0.00110275,0.0004133
7,-0.00713813,0.00301623,0.00031526,-0.00067431,-0.00100102,-
0.0000003
4,-0.02474987,-0.01393611,0.00978795,-0.00234389,-
0.00004128,0.0015687
8,0.00001132,-0.00076144,0.00069527,-0.00008802,0.00008139,-
0.00056071
,0.00025914,0.00007625,0.00000665,0.00011209,-0.00005910,-
0.00008842,-
0.00008302,0.00002010,-0.00006945,0.00005362,0.00001633,-0.00000908,-
0
.00000825,0.00041563,-
0.00028919,0.00000870,0.00009468,0.00009166,0.00
108222,-0.00018598,-0.00025207,-0.00038596,0.00037462,-0.00064645,-
0.0
0023060,-0.00057699,0.00016114,-0.00005726,0.00008314,-
0.00016015,0.00
000971,0.00030200,0.00002694,-0.00009708,0.00002907,-
0.00001369,0.0001
5371,-0.00027496,0.00016360,-0.00006943,-0.00001992,-0.00000637,-
0.000
66080,0.00030269,-0.00016039,0.00005601,-0.00001300,0.00000683,-
0.2490
9382,-0.51100270,0.21609820,0.02596153,0.01460123,-0.00976780,-
0.00922
791,-0.08134033,0.05129155,-0.00399908,-
0.00877743,0.00614979,0.271160
40,0.59711501,-0.00012061,-0.00014798,-
0.00030193,0.00061176,0.0003673

4,-0.00175770,0.00095024,-0.00013282,0.00132378,0.00106071,-
0.00011793
,-0.00079266,0.00065014,-0.00024350,0.00056503,0.00179667,-
0.00307654,
0.00316037,0.00049420,-0.00064728,-
0.00034307,0.01199822,0.01614133,0.
01086980,-0.00097391,-0.00112919,-0.00074562,-0.00047391,0.00101621,-
0
.00051978,0.00005596,-0.00042811,0.00080072,-0.00024598,-
0.00058526,0.
00015267,-0.00003595,0.00006608,0.00012006,0.00023863,0.00047560,-
0.00
032391,-0.00001544,-0.00006738,0.00001480,-0.00059118,-
0.00027629,0.00
059852,-0.00001233,-0.00009551,-0.00005357,-
0.00138196,0.00070962,0.00
017954,-0.00012074,-0.00064257,0.00058763,0.00056648,0.00016159,-
0.000
04932,0.00006421,-0.00004306,0.00007586,-0.00031008,-
0.00042190,0.0001
2967,0.00002185,-0.00002091,0.00001083,-0.00021293,0.00047847,-
0.00026
420,0.00001941,0.00000623,0.00000198,0.00073998,-
0.00025838,0.00009826
,-0.00004135,-0.00000092,0.00001782,0.12365916,0.21884468,-
0.17504479,
-0.01356049,-0.00406243,0.00988018,0.00340199,0.04891325,-
0.01212083,0
.00219586,0.00314502,-0.00370422,-0.13040685,-0.27832450,0.16733258,-
0
.00283360,0.00083598,0.00413381,-0.00092359,-
0.00040918,0.00028067,0.0
0014638,0.00001063,-0.00011592,0.00245887,-0.02238530,0.01250911,-
0.08
882552,0.00212328,0.00578032,0.00025158,-
0.00179411,0.00058419,0.00009
263,0.00053478,0.00034025,-0.00014149,-0.00004854,-0.00047040,-
0.00005
638,-0.00009549,-0.00009481,0.00011624,-0.00135277,0.00042205,-
0.00030
543,-0.00007725,0.00027968,-0.00002344,-0.00019550,-0.00006759,-
0.0000
0162,-0.00000499,0.00003381,0.00026266,-0.00031073,-
0.00010025,0.00005
485,0.00007116,0.00006342,-0.00126671,-0.00091334,0.00032161,-
0.000396
03,-0.00027606,0.00130443,0.00543802,0.02529141,-0.01409068,-
0.0061194
7,0.00183875,0.00068102,0.00062090,0.00151377,-0.00082300,-
0.00041067,
0.00036450,-0.00006739,-0.00004042,0.00021465,-0.00006549,-
0.00001800,

This journal is © The Royal Society of Chemistry 2014

0.00005199,-0.00001072,0.00049010,0.00023113,-0.00024625,-
0.00005263,-
0.00001238,0.00001136,-0.00129864,0.00057899,-0.00086306,-
0.00098724,0
.00116655,-0.00112503,0.00014538,-0.00036433,0.00034590,0.00001588,-
0.
00121326,0.00062730,-0.00000660,0.00030983,-0.00047750,-
0.00045400,0.0
0029808,-0.00024494,-0.00003519,0.00013909,-
0.00009703,0.59189944,0.00
265582,0.00278011,0.00027430,-0.00036689,-0.00211309,-0.00078262,-
0.00
004068,0.00010196,-0.00011616,-0.00738669,-
0.00227084,0.00819111,0.004
00207,-0.15868135,0.06233037,-0.00242105,-
0.00605020,0.00009423,0.0004
3564,0.00057291,0.00095866,-0.00036020,-0.00097606,-0.00029846,-
0.0001
0651,-0.00021476,-0.00002156,0.00018466,0.00034157,-
0.00036629,0.00012
666,0.00012050,-0.00009058,-0.00024724,0.00055630,-
0.00028806,0.000017
40,0.00003242,0.00000914,-0.00051605,-
0.00091342,0.00049589,0.00013218
,0.00005846,0.00004714,0.00214054,-0.00084086,-
0.00198620,0.00022999,0
.00044047,-0.00006373,0.00649969,-
0.01386151,0.00881778,0.00088510,0.0
0277799,0.00169115,-0.00033583,-
0.00003501,0.00004599,0.00003311,0.000
05576,-0.00002473,0.00014917,0.00035053,-
0.00033826,0.00000931,0.00002
423,-0.00000253,0.00015738,-0.00087404,0.00031657,-
0.00005909,0.000105
52,0.00010124,-0.00257696,-0.00019737,-
0.00036784,0.00033074,0.0001554
6,0.00023238,-0.00013742,0.00048281,-0.00040752,0.00227978,-
0.00108004
,0.00071182,-0.00041548,-0.00102584,0.00094181,-
0.00042514,0.00031263,
-0.00070372,-0.00035109,-0.00050496,0.00040135,-
0.00775531,0.48870184,
0.00518156,-0.00101265,0.00085963,-0.00032738,-0.00216718,-
0.00040971,
0.00002056,0.00025731,0.00005225,0.00291479,0.01939888,-
0.01104359,0.0
0517829,0.06723430,-0.11932913,-0.00098201,-0.00277207,0.00166049,-
0.0
0016564,-0.00051938,0.00033679,0.00017447,-0.00046675,-0.00032737,-
0.0
0018516,-0.00028891,0.00002567,-0.00022063,0.00123821,-
0.00032384,0.00

029432,0.00015957,-0.00011063,0.00008008,0.00014996,-
0.00034790,0.0000
3109,0.00007829,-0.00000520,-0.00058187,0.00075071,-
0.00021762,0.00008
202,0.00002447,0.00007787,-0.00085673,-0.00053299,-
0.00173635,0.000584
21,0.00101707,-0.00039248,-0.00265141,0.00797142,-0.00148731,-
0.001519
59,0.00032563,0.00365510,0.00030765,0.00038365,-0.00021927,-
0.00001631
,0.00013350,0.00006743,-0.00026148,0.00008382,-
0.00014795,0.00001090,0
.00009206,-0.00001611,0.00056656,0.00067567,-
0.00051055,0.00000282,0.0
0002741,0.00007816,-0.00035919,-0.00139248,-
0.00153644,0.00038384,0.00
106504,0.00003377,0.00025401,0.00015454,-0.00019865,0.00162792,-
0.0004
5662,0.00011584,-0.00035869,-0.00052068,0.00025687,-0.00125278,-
0.0003
7934,-0.00025588,-0.00032526,-0.00025224,0.00026998,-
0.00993815,0.0250
0163,0.54700183,-0.00008103,0.00052205,-0.00007576,0.00036694,-
0.00007
198,-0.00017810,0.00000264,0.00001677,0.00001754,-0.00010809,-
0.000354
86,0.00076233,-0.00070958,0.00101362,0.00046717,-
0.00043613,0.00003188
,-0.00016801,-0.00002805,-0.00016692,-0.00006438,0.00020794,-
0.0000459
2,0.00003604,-0.00001181,-
0.00002376,0.00001682,0.00006563,0.00004838,
-0.00008463,-0.00001498,0.00000695,-0.00000455,-
0.00001681,0.00010749,
-0.00004456,-0.00000253,0.00004273,-0.00002730,-
0.00018942,0.00018340,
0.00006828,-0.00002091,-0.00001658,0.00000779,0.00061620,-
0.00082661,0
.00010346,-0.00092619,0.00002240,-0.00000260,-0.00064946,0.00047106,-
0
.00062969,-0.00024210,-0.00050700,0.00012291,0.00010385,-
0.00002278,0.
00003373,-0.00000943,0.00000663,0.00001595,-0.00006141,-
0.00010564,0.0
0004340,0.00000040,-0.00002297,0.00001829,-0.00019233,0.00002657,-
0.00
006610,-0.00001436,0.00002549,0.00000898,0.00076764,0.00025988,-
0.0003
1264,-0.00025901,0.00009537,0.00034953,-0.00016158,0.00040774,-
0.00016
673,0.00032474,0.00063217,-0.00030338,-0.00007611,-
0.00045873,0.000421

49,0.00007860,-0.00044996,0.00001397,-0.00002043,-
0.00018248,0.0000885
9,-0.05635306,-0.04334132,-0.02973217,0.05758481,0.00068624,-
0.0003966
4,0.00069418,-0.00014447,-0.00062416,-
0.00027083,0.00005909,0.00010292
,0.00014574,0.00128813,0.00001731,-0.00049648,-0.00506553,-
0.02418855,
-0.01170036,-
0.00030439,0.00018544,0.00116442,0.00009527,0.00018090,0.
00012052,-0.00002274,-0.00025674,-0.00001637,-0.00011338,-
0.00012173,0
.00000177,0.00006173,0.00011147,-0.00010192,0.00001218,0.00001860,-
0.0
0000422,0.00000726,0.00006505,-0.00010324,-0.00001635,0.00002539,-
0.00
001736,-
0.00009755,0.00031479,0.00005072,0.00000595,0.00000385,0.00000
552,-0.00029735,0.00003271,0.00001988,-0.00038602,0.00015776,-
0.000079
55,-0.00127480,-0.00009195,0.00040961,-0.00027192,-
0.00014367,0.001067
15,-0.00007545,0.00008340,-0.00004745,0.00000983,0.00001087,-
0.0000020
8,-0.00000956,0.00007021,-0.00009181,0.00001524,0.00001919,-
0.00002132
,0.00024286,0.00018741,-0.00000659,0.00001130,-
0.00000216,0.00000502,0
.00008833,-0.00022713,-0.00008883,0.00043991,-0.00006758,-
0.00034578,0
.00032233,0.00010000,-0.00010108,0.00129642,-0.00054987,0.00041035,-
0.
00025978,-0.00010778,0.00011352,-0.00030868,0.00059678,-0.00025753,-
0.
00022758,-0.00017467,0.00013852,-0.04399270,-0.20921760,-
0.11739780,0.
04787238,0.23058451,-0.00056729,-0.00056038,-
0.00029735,0.00021689,0.0
0097730,0.00050611,-0.00002605,-0.00005561,-
0.00004262,0.00094641,0.00
006739,-0.00063407,0.00432895,0.01480716,0.01289364,0.00064524,-
0.0002
7686,-0.00021970,-0.00006650,0.00028496,0.00017016,-
0.00026259,0.00046
783,-0.00073290,0.00008984,0.00009208,0.00009467,-0.00013786,-
0.000049
08,0.00015530,-0.00002018,-0.00001775,0.00001199,0.00015742,-
0.0002680
4,0.00013597,-0.00000600,-0.00001038,-
0.00000871,0.00024235,0.00029634
,-0.00027386,-0.00002230,-0.00001677,-0.00002396,-0.00017527,-
0.000066

This journal is © The Royal Society of Chemistry 2014

62,0.00030790,0.00044657,0.00025668,-0.00022391,-
0.00065142,0.00033956
,-0.00024284,0.00015720,-0.00036158,-0.00062637,0.00009323,-
0.00006086
,0.00004505,0.00001133,-0.00001986,0.00000299,-0.00007807,-
0.00014584,
0.00014536,-0.00000316,-0.00000263,-0.00001079,-
0.00014736,0.00026902,
-0.00007762,0.00000647,-0.00002483,-0.00002754,0.00004346,-
0.00021967,
0.00035503,-0.00013527,0.00006758,-0.00015552,-
0.00024088,0.00014725,0
.00004151,-0.00086800,0.00114172,-0.00082701,0.00005319,-
0.00020154,0.
00026071,0.00006938,-0.00105383,0.00033441,0.00008564,-0.00001988,-
0.0
0004059,-0.02953916,-0.11215046,-
0.12633166,0.03307128,0.12560815,0.13
671233,-0.00011030,0.00054542,-0.00033839,-0.00001998,-0.00023116,-
0.0
0027796,0.00002404,0.00000572,0.00002295,-0.00049441,-
0.00028553,0.001
51387,0.00252437,0.00295448,-0.00010557,-0.00046933,0.00003183,-
0.0005
2453,-0.00006192,0.00016139,0.00014792,-0.00007872,-
0.00023249,0.00026
958,-0.00002624,-0.00000896,-0.00005238,0.00005575,0.00001613,-
0.00001
046,-0.00000968,-0.00001410,-0.00002597,-
0.00010344,0.00010239,0.00008
722,-0.00001665,-0.00002910,-0.00001459,0.00001684,-
0.00040929,0.00026
112,-0.00000294,0.00000882,0.00000655,-
0.00005339,0.00009820,0.0006243
1,-0.00036950,-0.00043242,0.00123686,0.00033102,-0.00124344,-
0.0002050
4,0.00023556,-0.00016428,-0.00020269,-
0.00007769,0.00005733,0.00003912
,0.00000830,-0.00000153,0.00001269,0.00001896,0.00010699,-
0.00000781,-
0.00000015,0.00003093,-0.00001096,0.00019623,0.00001180,-0.00008902,-
0
.00000702,-0.00001625,-0.00001805,-0.00045829,-
0.00026424,0.00011628,0
.00021921,0.00035902,-0.00004268,0.00001325,0.00007873,-
0.00003118,0.0
0111741,-0.00153853,0.00029402,-0.00014600,-0.00008403,0.00023085,-
0.0
0087737,0.00046515,-0.00022605,-0.00005452,-0.00008632,0.00004277,-
0.2
6614253,0.03367551,-0.10300861,-0.00493791,0.00033988,-
0.00140748,0.28

This journal is © The Royal Society of Chemistry 2014


```
 815039,-0.00028190,-0.00035463,-0.00035019,0.00003089,0.00003561,-
0.00
 020324,-0.00002103,-0.00001675,0.00005450,0.00038163,0.00064055,-
0.000
 73497,0.02729614,-0.00695248,0.01225082,-0.00037637,0.00069849,-
0.0002
 2223,0.00012168,-0.00004386,-0.00009604,-0.00011520,-
0.00015807,0.0005
 7076,-0.00004903,0.00002403,-0.00008242,0.00020593,-0.00000020,-
0.0000
 7370,0.00001576,-0.00000664,0.00000484,-0.00007669,0.00019644,-
0.00003
 245,0.00000094,-0.00000244,0.00000940,-0.00017679,-
0.00018197,0.000112
 97,0.00001239,0.00000498,0.00000401,-0.00015196,0.00058997,-
0.00017275
 ,0.00005704,0.00034832,-0.00015510,-0.00189692,-
0.00364292,0.00326087,
 0.00167718,-0.00044045,-0.00026045,-0.00026278,-
0.00044407,0.00014044,
 0.00011803,-0.00011041,0.00000484,-
0.00004771,0.00001553,0.00001763,0.
 00001133,0.00000196,-
0.00002201,0.00009367,0.00020532,0.00001549,0.000
 03448,-0.00001613,0.00000352,-0.00047664,-0.00026646,0.00033988,-
0.000
 03153,0.00011436,-0.00029606,0.00047167,-
0.00058027,0.00021999,0.00091
 112,-0.00444150,0.00136093,-0.00008077,0.00095663,-0.00068962,-
0.00023
 664,0.00239363,-0.00031919,-0.00004568,0.00027624,-
0.00012178,0.031447
 53,-0.05053019,0.01601978,-0.02475879,0.00449626,-0.01075816,-
0.036232

17,0.05836950,0.00012320,0.00008980,0.00034149,0.00000792,0.00017651,0
 .00019672,0.00001034,-0.00004420,-0.00009259,-
0.00021202,0.00017395,0.
 00057954,-0.01660845,0.00215625,-0.00789495,-0.00035194,-0.00047981,-
0
 .00039997,0.00016417,0.00005943,0.00010463,-0.00000649,0.00012893,-
0.0
 0031584,0.00000958,0.00002746,0.00001098,-0.00015422,-
0.00018469,0.000
 10889,-0.00000441,-0.00001135,0.00002356,-0.00002349,-
0.00017832,0.000
 01046,-0.00000276,-0.00006304,0.00003793,0.00032854,-0.00024616,-
0.000
 01908,0.00000535,0.00001849,0.00001035,-0.00023371,0.00091001,-
0.00047
 889,0.00094215,-0.00069357,-0.00124541,0.00142096,0.00210907,-
0.001605
```

95,-0.00091551,0.00014407,0.00047531,0.00018446,0.00011315,-
0.00011812
,-0.00006017,0.00004619,-0.00001720,0.00001615,-0.00011225,-
0.00002877
,-0.00001108,-0.00003049,0.00002290,-0.00024686,-
0.00007119,0.00014712
,-0.00001770,0.00002517,0.00001414,0.00107317,0.00018992,-
0.00002879,-
0.00021858,-0.00046418,0.00001142,0.00004357,-
0.00008047,0.00015698,0.
00043598,-0.00147225,0.00117886,0.00003276,0.00044959,-0.00028101,-
0.0
0023811,0.00058412,-0.00098617,0.00004976,0.00012489,-0.00010947,-
0.10
263440,0.01809168,-0.09861762,-0.01637640,0.00250604,-
0.00814058,0.111
03408,-
0.02055956,0.10481791,0.00014934,0.00016163,0.00021994,0.000054
75,0.00008891,0.00000831,0.00000112,-0.00002743,-
0.00002948,0.00064393
,0.00054454,0.00012808,0.00016409,-0.00218981,-0.00066802,-
0.00043168,
0.00030856,0.00006852,0.00016041,-0.00045146,-0.00023746,0.00028200,-
0
.00003069,0.00004973,-0.00001257,-0.00000768,-0.00000097,-
0.00005685,-
0.00009080,0.00002951,-0.00001849,-0.00000760,-0.00000729,-
0.00002955,
-0.00008655,-0.00000663,-0.00001105,-
0.00003393,0.00001487,0.00021873,
-0.00008082,0.00004102,0.00000083,0.00001593,0.00001884,-
0.00027306,0.
00040350,0.00015598,0.00003248,-0.00048757,-0.00014472,-
0.00070427,0.0
0019046,-0.00056524,0.00008088,-0.00034008,0.00020876,0.00000015,-
0.00
008535,0.00003223,0.00001841,-0.00000285,0.00003279,-0.00009586,-
0.000
01922,-
0.00002908,0.00000706,0.00000757,0.00001814,0.00003885,0.000248
94,-0.00016373,0.00000897,-0.00000439,0.00000054,-
0.00088564,0.0006070
2,-0.00102170,-0.00178849,0.00122174,-0.00151342,0.00003806,-
0.0000016
7,0.00002638,-0.00012007,-
0.00021264,0.00019490,0.00010759,0.00019450,
-0.00015297,0.00018090,0.00000652,-0.00043811,0.00004408,0.00005865,-
0
.00005608,-0.17530069,0.01289820,0.13504798,0.00540332,0.00001393,-
0.0
0631001,-0.01839337,0.00243119,0.02243416,0.19048567,-
0.00142799,0.000

29941,0.00077254,-0.00008622,0.00013005,-0.00001781,0.00003619,-
0.0000
2343,0.00001724,0.00190894,-0.00443904,0.00250551,-
0.02213294,0.000635
72,0.02166574,-0.00027846,0.00049300,0.00041604,0.00000676,-
0.00044650
,-0.00037829,0.00021836,-0.00015603,0.00016645,-0.00003122,-
0.00001404
,-0.00002734,0.00006615,-0.00048426,0.00002107,-0.00013158,-
0.00004754
,0.00007592,0.00008668,-0.00002037,0.00001013,-
0.00001441,0.00002906,-
0.00001922,-0.00009112,0.00032791,-0.00001022,-0.00003963,-
0.00001192,
0.00001392,0.00063576,-0.00072396,0.00003382,-0.00017413,0.00036139,-
0
.00027815,-0.00048622,0.00088953,-0.00040469,-0.00020744,-
0.00025443,-
0.00029236,-0.00016500,0.00013935,0.00000191,-0.00002306,0.00000562,-
0
.00001111,0.00015464,0.00015993,-0.00008345,-
0.00000092,0.00000601,0.0
0000290,0.00016873,-0.00035996,0.00002821,-
0.00000845,0.00002247,0.000
03208,0.00046078,0.00043545,-
0.00014957,0.00065262,0.00003557,0.000564
79,-0.00001293,-0.00007819,-0.00000182,-0.00008928,-0.00007943,-
0.0000
1085,0.00015444,0.00010556,-0.00005973,0.00007628,0.00010292,-
0.000020
52,0.00004931,0.00006227,-0.00002102,0.01417916,-0.04858433,-
0.0140838
4,0.01956335,-0.00119460,-0.01848240,0.00222412,-0.00117835,-
0.0034332
1,-0.01524126,0.05385516,0.00116923,-0.00043031,-
0.00022876,0.00021197
,0.00018474,0.00029227,-0.00008178,-0.00001311,-0.00006159,-
0.00106401
,0.00325800,-0.00075010,0.01220399,-0.00273125,-
0.01316255,0.00004018,
-0.00067799,0.00024801,0.00007344,0.00015405,0.00031970,-
0.00035555,0.
00019326,-0.00049436,0.00006270,0.00005572,0.00009232,-
0.00020952,0.00
030086,-0.00009611,0.00007256,0.00003100,-0.00006241,-0.00002276,-
0.00
009665,0.00003259,0.00001179,-0.00000850,-
0.00000378,0.00014813,0.0000
0342,-0.00002423,0.00002604,0.00000178,-0.00001537,-
0.00063358,0.00030
173,0.00037343,-0.00014356,-0.00017191,-0.00006450,0.00059276,-
0.00046

331,0.00059314,0.00004231,0.00023733,0.00019745,0.00011443,-
0.00022989
,0.00006682,0.00000097,-0.00002495,0.00000170,0.00001457,-
0.00019483,0
.00002070,-0.00000663,-0.00008142,0.00003418,-0.00045263,-
0.00032362,0
.00027400,0.00000208,0.00003319,0.00001677,0.00065719,0.00087443,-
0.00
017885,-0.00140471,-0.00034240,-0.00013234,0.00000502,-
0.00009332,0.00
002670,-0.00035270,0.00007761,-0.00006678,-0.00004384,0.00010282,-
0.00
002147,0.00011771,-0.00014179,-0.00000238,0.00000849,0.00005477,-
0.000
01840,0.13335284,-0.01074553,-0.19092646,0.01256943,-0.00131050,-
0.013
23555,-0.00934078,0.00075925,0.01213121,-
0.14738578,0.01145734,0.20482
501\\0.00000337,-0.00000200,0.00000740,-0.00000398,-0.00000270,-
0.0000
0270,0.00000159,-0.00000096,-
0.00000198,0.00000048,0.00000127,0.000000
57,-0.00000358,0.00000669,-0.00000519,-
0.00000131,0.00000714,0.0000047
4,-0.00000389,0.00000233,-0.00000132,0.00000266,-0.00000235,-
0.0000053
7,-0.00000351,0.,-
0.00000387,0.00000185,0.00000120,0.00000345,0.000004
28,-0.00000116,0.00000344,0.00000484,-
0.00000199,0.00000598,0.00000545
,-0.00000172,0.00000743,0.00000307,-
0.00000129,0.00000500,0.00000320,-
0.00000080,0.00000800,0.00000149,0.00000129,0.00000478,0.00000143,-
0.0
0000282,0.00000609,0.00000132,-0.00000351,-
0.00000283,0.00000289,0.000
00111,-0.00000298,-0.00000004,-0.00000002,-0.00000476,0.00000295,-
0.00
000125,-0.00000666,0.00000205,0.00000225,-0.00000824,0.00000102,-
0.000
00040,-0.00000978,0.00000047,-0.00000125,-0.00000719,-
0.00000063,0.000
00020,-0.00000903,-0.00000101,-0.00000003,-0.00000570,-
0.00000170,0.00
000042,-0.00000379,-0.00000058,0.00000256,0.00000788,-
0.00000174,0.000
00167,0.00000173,-0.00000236,0.00000055,0.00000394,-
0.00000511,0.00000
568,0.00000519,-0.00000154,-0.00000138,0.00000171,-0.00000429,-
0.00000
990,0.00000228,0.00000031,0.00000228,0.00000292,-0.00000676,-
0.0000011

This journal is © The Royal Society of Chemistry 2014

```
 7,0.00000062,-0.00000267,0.00000007,-0.00000173\\\@


 WHEN ALL ELSE FAILS, LOOK AT THE SCHRODINGER EQUATION.
     -- RUSSELL T. PACK, APRIL 1978
 Job cpu time:  0 days 10 hours 43 minutes 15.8 seconds.
 File lengths (MBytes):  RWF=    765 Int=      0 D2E=      0 Chk=
13 Scr=      1
 Normal termination of Gaussian 09 at Fri Oct 19 00:43:23 2012.
```

This journal is © The Royal Society of Chemistry 2014

(15S) 9-methyl-9,10,11,15-tetrahydro-9,10-[3,4]furanoanthracene-12,14-dione-

```
Entering Link 1 = C:\G09W\l1.exe PID=      6352.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2009, Gaussian, Inc.
                    All Rights Reserved.

 This is part of the Gaussian(R) 09 program.  It is based on
 the Gaussian(R) 03 system (copyright 2003, Gaussian, Inc.),
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,
 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be
 used, copied, transmitted, or stored only in accord with that
 written license.

 The following legend is applicable only to US Government
 contracts under FAR:

                       RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is
 subject to restrictions as set forth in subparagraphs (a)
 and (c) of the Commercial Computer Software - Restricted
 Rights clause in FAR 52.227-19.

 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ----------------------------------------------------------------
 Warning -- This program may not be used in any manner that
 competes with the business of Gaussian, Inc. or will provide
 assistance to any competitor of Gaussian, Inc.  The licensee
 of this program is prohibited from giving any competitor of
 Gaussian, Inc. access to this program.  By using this program,
 the user acknowledges that Gaussian, Inc. is engaged in the
 business of creating and licensing software in the field of
 computational chemistry and represents and warrants to the
```

This journal is © The Royal Society of Chemistry 2014

```
 licensee that it is not a competitor of Gaussian, Inc. and that
 it will not use this program in any manner prohibited above.
 ----------------------------------------------------------------


 Cite this work as:
 Gaussian 09, Revision A.02,
 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
 M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
 G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
 A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
 M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
 Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
 J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
 K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand,
 K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
 M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
 V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
 O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
 R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
 P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
 O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
 and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

 ******************************************
 Gaussian 09:  IA32W-G09RevA.02 11-Jun-2009
                24-Jul-2013
 ******************************************
 %mem=64MW
 %chk=F:\solid state\Mack group papers\Ball mill energetics\James
Calculations\Me
 thylAnthracene\9METHYLANTHRACENEPRODUCT2.chk
 ---------------------------------------
 # opt b3lyp/6-31+g(d) geom=connectivity
 ---------------------------------------
 1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
 2/9=110,12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
 4//1;
 5/5=2,38=5/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 7//1,2,3,16;
 1/14=-1,18=20,19=15/3(2);
 2/9=110/2;
 99//99;
 2/9=110/2;
 3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
 4/5=5,16=3/1;
 5/5=2,38=5/2;
 7//1,2,3,16;
 1/14=-1,18=20,19=15/3(-5);
 2/9=110/2;
```

This journal is © The Royal Society of Chemistry 2014

```
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 -------------------
 9-methylnanthracene
 -------------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                     1.71268  -0.04654  -0.89377
 C                     0.30521  -0.05671  -1.45643
 H                     0.27672  -0.00083  -2.54731
 C                     1.7531   -0.10217   0.51129
 C                    -0.32354  -1.40489  -0.96262
 H                     0.21778  -2.23909  -1.41907
 C                    -0.4688    1.06686  -0.79259
 C                    -0.4311    1.02603   0.61362
 C                     0.37094  -0.1516    1.1811
 C                    -0.30927  -1.45392   0.57753
 H                     0.2254   -2.3271    0.96525
 C                    -1.18206   2.06234  -1.45384
 H                    -1.21397   2.07964  -2.54034
 C                    -1.11205   1.99347   1.35
 H                    -1.10019   1.97166   2.43519
 C                    -1.81928   3.00094   0.68395
 H                    -2.34553   3.757     1.26008
 C                    -1.85595   3.03612  -0.70971
 H                    -2.41048   3.8185   -1.22028
 C                     2.88727  -0.00598  -1.63746
 H                     2.84451   0.03528  -2.72337
 C                     4.12135  -0.01158  -0.97786
 H                     5.0425    0.02723  -1.55278
 C                     4.1675   -0.06445   0.41445
 H                     5.12598  -0.06641   0.92637
 C                     2.98471  -0.11312   1.16247
 H                     3.03783  -0.15332   2.24597
 C                    -1.79047  -1.52354  -1.34169
 C                    -1.77988  -1.60407   0.95398
 O                    -2.56377  -1.63333  -0.19354
 O                    -2.27525  -1.70342   2.04067
 O                    -2.28181  -1.52483  -2.43352
 C                     0.42569  -0.20423   2.70695
 H                     0.99915  -1.07477   3.043
 H                    -0.57608  -0.28685   3.13322
 H                     0.90663   0.69379   3.10899


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Initialization pass.
                           ----------------------------
                           !    Initial Parameters    !
```

This journal is © The Royal Society of Chemistry 2014

! (Angstroms and Degrees) !

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.5158	estimate D2E/DX2
R2	R(1,4)	1.4067	estimate D2E/DX2
R3	R(1,20)	1.3908	estimate D2E/DX2
R4	R(2,3)	1.0927	estimate D2E/DX2
R5	R(2,5)	1.5674	estimate D2E/DX2
R6	R(2,7)	1.5173	estimate D2E/DX2
R7	R(4,9)	1.5367	estimate D2E/DX2
R8	R(4,26)	1.3932	estimate D2E/DX2
R9	R(5,6)	1.0942	estimate D2E/DX2
R10	R(5,10)	1.541	estimate D2E/DX2
R11	R(5,28)	1.5198	estimate D2E/DX2
R12	R(7,8)	1.4073	estimate D2E/DX2
R13	R(7,12)	1.3918	estimate D2E/DX2
R14	R(8,9)	1.5337	estimate D2E/DX2
R15	R(8,14)	1.3935	estimate D2E/DX2
R16	R(9,10)	1.5884	estimate D2E/DX2
R17	R(9,33)	1.5277	estimate D2E/DX2
R18	R(10,11)	1.0948	estimate D2E/DX2
R19	R(10,29)	1.5254	estimate D2E/DX2
R20	R(12,13)	1.0871	estimate D2E/DX2
R21	R(12,18)	1.3986	estimate D2E/DX2
R22	R(14,15)	1.0855	estimate D2E/DX2

This journal is © The Royal Society of Chemistry 2014

```
 ! R23   R(14,16)              1.3996         estimate D2E/DX2
!
 ! R24   R(16,17)              1.0865         estimate D2E/DX2
!
 ! R25   R(16,18)              1.3946         estimate D2E/DX2
!
 ! R26   R(18,19)              1.0864         estimate D2E/DX2
!
 ! R27   R(20,21)              1.0875         estimate D2E/DX2
!
 ! R28   R(20,22)              1.3993         estimate D2E/DX2
!
 ! R29   R(22,23)              1.0865         estimate D2E/DX2
!
 ! R30   R(22,24)              1.3941         estimate D2E/DX2
!
 ! R31   R(24,25)              1.0866         estimate D2E/DX2
!
 ! R32   R(24,26)              1.4003         estimate D2E/DX2
!
 ! R33   R(26,27)              1.0856         estimate D2E/DX2
!
 ! R34   R(28,30)              1.3886         estimate D2E/DX2
!
 ! R35   R(28,32)              1.1973         estimate D2E/DX2
!
 ! R36   R(29,30)              1.39           estimate D2E/DX2
!
 ! R37   R(29,31)              1.1984         estimate D2E/DX2
!
 ! R38   R(33,34)              1.0953         estimate D2E/DX2
!
 ! R39   R(33,35)              1.0918         estimate D2E/DX2
!
 ! R40   R(33,36)              1.0952         estimate D2E/DX2
!
 ! A1    A(2,1,4)            113.4015         estimate D2E/DX2
!
 ! A2    A(2,1,20)           125.8652         estimate D2E/DX2
!
 ! A3    A(4,1,20)           120.7278         estimate D2E/DX2
!
 ! A4    A(1,2,3)            113.2322         estimate D2E/DX2
!
 ! A5    A(1,2,5)            105.1467         estimate D2E/DX2
!
 ! A6    A(1,2,7)            107.8361         estimate D2E/DX2
!
 ! A7    A(3,2,5)            110.3683         estimate D2E/DX2
!
 ! A8    A(3,2,7)            112.683          estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A9    A(5,2,7)              107.1249         estimate D2E/DX2
!
 ! A10   A(1,4,9)              114.2537         estimate D2E/DX2
!
 ! A11   A(1,4,26)             119.5084         estimate D2E/DX2
!
 ! A12   A(9,4,26)             126.2374         estimate D2E/DX2
!
 ! A13   A(2,5,6)              109.0183         estimate D2E/DX2
!
 ! A14   A(2,5,10)             109.7876         estimate D2E/DX2
!
 ! A15   A(2,5,28)             112.0716         estimate D2E/DX2
!
 ! A16   A(6,5,10)             112.836          estimate D2E/DX2
!
 ! A17   A(6,5,28)             108.2976         estimate D2E/DX2
!
 ! A18   A(10,5,28)            104.8176         estimate D2E/DX2
!
 ! A19   A(2,7,8)              113.7049         estimate D2E/DX2
!
 ! A20   A(2,7,12)             125.6776         estimate D2E/DX2
!
 ! A21   A(8,7,12)             120.6126         estimate D2E/DX2
!
 ! A22   A(7,8,9)              113.955          estimate D2E/DX2
!
 ! A23   A(7,8,14)             119.6556         estimate D2E/DX2
!
 ! A24   A(9,8,14)             126.377          estimate D2E/DX2
!
 ! A25   A(4,9,8)              106.5218         estimate D2E/DX2
!
 ! A26   A(4,9,10)             104.2363         estimate D2E/DX2
!
 ! A27   A(4,9,33)             113.8415         estimate D2E/DX2
!
 ! A28   A(8,9,10)             105.3676         estimate D2E/DX2
!
 ! A29   A(8,9,33)             114.5037         estimate D2E/DX2
!
 ! A30   A(10,9,33)            111.5074         estimate D2E/DX2
!
 ! A31   A(5,10,9)             110.9562         estimate D2E/DX2
!
 ! A32   A(5,10,11)            112.5716         estimate D2E/DX2
!
 ! A33   A(5,10,29)            103.9371         estimate D2E/DX2
!
 ! A34   A(9,10,11)            108.0718         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A35   A(9,10,29)            113.5642         estimate D2E/DX2
!
 ! A36   A(11,10,29)           107.7526         estimate D2E/DX2
!
 ! A37   A(7,12,13)            120.0844         estimate D2E/DX2
!
 ! A38   A(7,12,18)            119.4823         estimate D2E/DX2
!
 ! A39   A(13,12,18)           120.4333         estimate D2E/DX2
!
 ! A40   A(8,14,15)            120.5977         estimate D2E/DX2
!
 ! A41   A(8,14,16)            119.6825         estimate D2E/DX2
!
 ! A42   A(15,14,16)           119.7197         estimate D2E/DX2
!
 ! A43   A(14,16,17)           119.5589         estimate D2E/DX2
!
 ! A44   A(14,16,18)           120.4663         estimate D2E/DX2
!
 ! A45   A(17,16,18)           119.9743         estimate D2E/DX2
!
 ! A46   A(12,18,16)           120.0966         estimate D2E/DX2
!
 ! A47   A(12,18,19)           119.8215         estimate D2E/DX2
!
 ! A48   A(16,18,19)           120.0817         estimate D2E/DX2
!
 ! A49   A(1,20,21)            120.1203         estimate D2E/DX2
!
 ! A50   A(1,20,22)            119.5143         estimate D2E/DX2
!
 ! A51   A(21,20,22)           120.3646         estimate D2E/DX2
!
 ! A52   A(20,22,23)           119.8756         estimate D2E/DX2
!
 ! A53   A(20,22,24)           120.0085         estimate D2E/DX2
!
 ! A54   A(23,22,24)           120.1158         estimate D2E/DX2
!
 ! A55   A(22,24,25)           119.9857         estimate D2E/DX2
!
 ! A56   A(22,24,26)           120.4543         estimate D2E/DX2
!
 ! A57   A(25,24,26)           119.5599         estimate D2E/DX2
!
 ! A58   A(4,26,24)            119.7849         estimate D2E/DX2
!
 ! A59   A(4,26,27)            120.6684         estimate D2E/DX2
!
 ! A60   A(24,26,27)           119.5457         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A61   A(5,28,30)            109.7226         estimate D2E/DX2
!
 ! A62   A(5,28,32)            128.5837         estimate D2E/DX2
!
 ! A63   A(30,28,32)           121.6931         estimate D2E/DX2
!
 ! A64   A(10,29,30)           109.9999         estimate D2E/DX2
!
 ! A65   A(10,29,31)           129.0831         estimate D2E/DX2
!
 ! A66   A(30,29,31)           120.9126         estimate D2E/DX2
!
 ! A67   A(28,30,29)           111.522          estimate D2E/DX2
!
 ! A68   A(9,33,34)            110.6453         estimate D2E/DX2
!
 ! A69   A(9,33,35)            111.0796         estimate D2E/DX2
!
 ! A70   A(9,33,36)            110.7411         estimate D2E/DX2
!
 ! A71   A(34,33,35)           107.4852         estimate D2E/DX2
!
 ! A72   A(34,33,36)           108.009          estimate D2E/DX2
!
 ! A73   A(35,33,36)           108.7632         estimate D2E/DX2
!
 ! D1    D(4,1,2,3)            179.2809         estimate D2E/DX2
!
 ! D2    D(4,1,2,5)             -60.1486        estimate D2E/DX2
!
 ! D3    D(4,1,2,7)              53.9028        estimate D2E/DX2
!
 ! D4    D(20,1,2,3)             -1.5706        estimate D2E/DX2
!
 ! D5    D(20,1,2,5)            118.9999        estimate D2E/DX2
!
 ! D6    D(20,1,2,7)           -126.9487        estimate D2E/DX2
!
 ! D7    D(2,1,4,9)              -0.3987        estimate D2E/DX2
!
 ! D8    D(2,1,4,26)            179.365         estimate D2E/DX2
!
 ! D9    D(20,1,4,9)           -179.596         estimate D2E/DX2
!
 ! D10   D(20,1,4,26)             0.1677        estimate D2E/DX2
!
 ! D11   D(2,1,20,21)             0.8096        estimate D2E/DX2
!
 ! D12   D(2,1,20,22)          -179.5239        estimate D2E/DX2
!
 ! D13   D(4,1,20,21)           179.9006        estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D14   D(4,1,20,22)          -0.433          estimate D2E/DX2
!
 ! D15   D(1,2,5,6)           -65.0777         estimate D2E/DX2
!
 ! D16   D(1,2,5,10)           58.9969         estimate D2E/DX2
!
 ! D17   D(1,2,5,28)          175.0477         estimate D2E/DX2
!
 ! D18   D(3,2,5,6)            57.3619         estimate D2E/DX2
!
 ! D19   D(3,2,5,10)         -178.5635         estimate D2E/DX2
!
 ! D20   D(3,2,5,28)           -62.5127        estimate D2E/DX2
!
 ! D21   D(7,2,5,6)          -179.6251         estimate D2E/DX2
!
 ! D22   D(7,2,5,10)           -55.5505        estimate D2E/DX2
!
 ! D23   D(7,2,5,28)            60.5002        estimate D2E/DX2
!
 ! D24   D(1,2,7,8)            -53.4776        estimate D2E/DX2
!
 ! D25   D(1,2,7,12)           127.3185         estimate D2E/DX2
!
 ! D26   D(3,2,7,8)          -179.1814         estimate D2E/DX2
!
 ! D27   D(3,2,7,12)             1.6147         estimate D2E/DX2
!
 ! D28   D(5,2,7,8)             59.2504         estimate D2E/DX2
!
 ! D29   D(5,2,7,12)         -119.9535         estimate D2E/DX2
!
 ! D30   D(1,4,9,8)            -52.5272         estimate D2E/DX2
!
 ! D31   D(1,4,9,10)            58.6            estimate D2E/DX2
!
 ! D32   D(1,4,9,33)         -179.6883         estimate D2E/DX2
!
 ! D33   D(26,4,9,8)           127.7277         estimate D2E/DX2
!
 ! D34   D(26,4,9,10)        -121.145          estimate D2E/DX2
!
 ! D35   D(26,4,9,33)            0.5666         estimate D2E/DX2
!
 ! D36   D(1,4,26,24)            0.2038         estimate D2E/DX2
!
 ! D37   D(1,4,26,27)          179.8511         estimate D2E/DX2
!
 ! D38   D(9,4,26,24)          179.9367         estimate D2E/DX2
!
 ! D39   D(9,4,26,27)           -0.416          estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D40   D(2,5,10,9)            -1.6217         estimate D2E/DX2
!
 ! D41   D(2,5,10,11)         -122.8826         estimate D2E/DX2
!
 ! D42   D(2,5,10,29)          120.7982         estimate D2E/DX2
!
 ! D43   D(6,5,10,9)           120.1998         estimate D2E/DX2
!
 ! D44   D(6,5,10,11)           -1.061          estimate D2E/DX2
!
 ! D45   D(6,5,10,29)         -117.3803         estimate D2E/DX2
!
 ! D46   D(28,5,10,9)         -122.1695         estimate D2E/DX2
!
 ! D47   D(28,5,10,11)         116.5696         estimate D2E/DX2
!
 ! D48   D(28,5,10,29)           0.2504         estimate D2E/DX2
!
 ! D49   D(2,5,28,30)         -119.1618         estimate D2E/DX2
!
 ! D50   D(2,5,28,32)           60.5562         estimate D2E/DX2
!
 ! D51   D(6,5,28,30)          120.5435         estimate D2E/DX2
!
 ! D52   D(6,5,28,32)          -59.7385         estimate D2E/DX2
!
 ! D53   D(10,5,28,30)          -0.1404         estimate D2E/DX2
!
 ! D54   D(10,5,28,32)         179.5777         estimate D2E/DX2
!
 ! D55   D(2,7,8,9)             -0.5944         estimate D2E/DX2
!
 ! D56   D(2,7,8,14)          -179.3937         estimate D2E/DX2
!
 ! D57   D(12,7,8,9)           178.6542         estimate D2E/DX2
!
 ! D58   D(12,7,8,14)           -0.1451         estimate D2E/DX2
!
 ! D59   D(2,7,12,13)           -0.2058         estimate D2E/DX2
!
 ! D60   D(2,7,12,18)          179.7393         estimate D2E/DX2
!
 ! D61   D(8,7,12,13)         -179.3588         estimate D2E/DX2
!
 ! D62   D(8,7,12,18)           0.5863         estimate D2E/DX2
!
 ! D63   D(7,8,9,4)            52.9541         estimate D2E/DX2
!
 ! D64   D(7,8,9,10)           -57.3834         estimate D2E/DX2
!
 ! D65   D(7,8,9,33)           179.7203         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D66   D(14,8,9,4)          -128.342          estimate D2E/DX2
!
 ! D67   D(14,8,9,10)          121.3206         estimate D2E/DX2
!
 ! D68   D(14,8,9,33)           -1.5758         estimate D2E/DX2
!
 ! D69   D(7,8,14,15)          179.4813         estimate D2E/DX2
!
 ! D70   D(7,8,14,16)           -0.4166         estimate D2E/DX2
!
 ! D71   D(9,8,14,15)            0.8442         estimate D2E/DX2
!
 ! D72   D(9,8,14,16)         -179.0536         estimate D2E/DX2
!
 ! D73   D(4,9,10,5)           -55.2239         estimate D2E/DX2
!
 ! D74   D(4,9,10,11)           68.647          estimate D2E/DX2
!
 ! D75   D(4,9,10,29)         -171.8661         estimate D2E/DX2
!
 ! D76   D(8,9,10,5)            56.7386         estimate D2E/DX2
!
 ! D77   D(8,9,10,11)         -179.3905         estimate D2E/DX2
!
 ! D78   D(8,9,10,29)          -59.9036         estimate D2E/DX2
!
 ! D79   D(33,9,10,5)         -178.4677         estimate D2E/DX2
!
 ! D80   D(33,9,10,11)         -54.5967         estimate D2E/DX2
!
 ! D81   D(33,9,10,29)          64.8901         estimate D2E/DX2
!
 ! D82   D(4,9,33,34)          -57.9554         estimate D2E/DX2
!
 ! D83   D(4,9,33,35)         -177.2525         estimate D2E/DX2
!
 ! D84   D(4,9,33,36)           61.7778         estimate D2E/DX2
!
 ! D85   D(8,9,33,34)          179.1488         estimate D2E/DX2
!
 ! D86   D(8,9,33,35)           59.8517         estimate D2E/DX2
!
 ! D87   D(8,9,33,36)          -61.118          estimate D2E/DX2
!
 ! D88   D(10,9,33,34)          59.6338         estimate D2E/DX2
!
 ! D89   D(10,9,33,35)         -59.6633         estimate D2E/DX2
!
 ! D90   D(10,9,33,36)         179.367          estimate D2E/DX2
!
 ! D91   D(5,10,29,30)          -0.2921         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D92   D(5,10,29,31)         178.9346         estimate D2E/DX2
!
 ! D93   D(9,10,29,30)         120.3891         estimate D2E/DX2
!
 ! D94   D(9,10,29,31)         -60.3842         estimate D2E/DX2
!
 ! D95   D(11,10,29,30)       -119.9423         estimate D2E/DX2
!
 ! D96   D(11,10,29,31)         59.2844         estimate D2E/DX2
!
 ! D97   D(7,12,18,16)          -0.4658         estimate D2E/DX2
!
 ! D98   D(7,12,18,19)         179.7076         estimate D2E/DX2
!
 ! D99   D(13,12,18,16)        179.4791         estimate D2E/DX2
!
 ! D100  D(13,12,18,19)         -0.3474         estimate D2E/DX2
!
 ! D101  D(8,14,16,17)        -179.7065         estimate D2E/DX2
!
 ! D102  D(8,14,16,18)           0.5377         estimate D2E/DX2
!
 ! D103  D(15,14,16,17)          0.3947         estimate D2E/DX2
!
 ! D104  D(15,14,16,18)       -179.3611         estimate D2E/DX2
!
 ! D105  D(14,16,18,12)         -0.0946         estimate D2E/DX2
!
 ! D106  D(14,16,18,19)        179.7315         estimate D2E/DX2
!
 ! D107  D(17,16,18,12)       -179.8494         estimate D2E/DX2
!
 ! D108  D(17,16,18,19)         -0.0233         estimate D2E/DX2
!
 ! D109  D(1,20,22,23)        -179.558          estimate D2E/DX2
!
 ! D110  D(1,20,22,24)           0.3268         estimate D2E/DX2
!
 ! D111  D(21,20,22,23)          0.1076         estimate D2E/DX2
!
 ! D112  D(21,20,22,24)        179.9925         estimate D2E/DX2
!
 ! D113  D(20,22,24,25)       -179.8548         estimate D2E/DX2
!
 ! D114  D(20,22,24,26)          0.0424         estimate D2E/DX2
!
 ! D115  D(23,22,24,25)          0.0297         estimate D2E/DX2
!
 ! D116  D(23,22,24,26)        179.9269         estimate D2E/DX2
!
 ! D117  D(22,24,26,4)          -0.3089         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D118  D(22,24,26,27)       -179.9602         estimate D2E/DX2
!
 ! D119  D(25,24,26,4)         179.5887         estimate D2E/DX2
!
 ! D120  D(25,24,26,27)         -0.0626         estimate D2E/DX2
!
 ! D121  D(5,28,30,29)          -0.0453         estimate D2E/DX2
!
 ! D122  D(32,28,30,29)       -179.7863         estimate D2E/DX2
!
 ! D123  D(10,29,30,28)          0.2187         estimate D2E/DX2
!
 ! D124  D(31,29,30,28)       -179.0817         estimate D2E/DX2
!
 ---------------------------------------------------------------------
-----------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
 Number of steps in this run= 216 maximum allowed number of steps=
216.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.712680   -0.046539   -0.893769
      2          6           0        0.305214   -0.056705   -1.456434
      3          1           0        0.276720   -0.000834   -2.547309
      4          6           0        1.753103   -0.102166    0.511289
      5          6           0       -0.323538   -1.404887   -0.962616
      6          1           0        0.217784   -2.239085   -1.419072
      7          6           0       -0.468801    1.066857   -0.792588
      8          6           0       -0.431095    1.026028    0.613616
      9          6           0        0.370938   -0.151602    1.181097
     10          6           0       -0.309273   -1.453917    0.577530
     11          1           0        0.225396   -2.327098    0.965246
     12          6           0       -1.182061    2.062340   -1.453836
     13          1           0       -1.213966    2.079635   -2.540335
     14          6           0       -1.112047    1.993470    1.349996
     15          1           0       -1.100189    1.971660    2.435190
     16          6           0       -1.819275    3.000935    0.683946
     17          1           0       -2.345529    3.757000    1.260075
     18          6           0       -1.855949    3.036120   -0.709708
     19          1           0       -2.410482    3.818503   -1.220277
     20          6           0        2.887271   -0.005975   -1.637461
     21          1           0        2.844512    0.035276   -2.723371
     22          6           0        4.121349   -0.011581   -0.977860
     23          1           0        5.042496    0.027225   -1.552778
     24          6           0        4.167501   -0.064452    0.414453
```

This journal is © The Royal Society of Chemistry 2014

25	1	0	5.125979	-0.066405	0.926373
26	6	0	2.984708	-0.113117	1.162466
27	1	0	3.037833	-0.153316	2.245974
28	6	0	-1.790467	-1.523535	-1.341687
29	6	0	-1.779877	-1.604069	0.953982
30	8	0	-2.563774	-1.633326	-0.193539
31	8	0	-2.275248	-1.703419	2.040665
32	8	0	-2.281813	-1.524832	-2.433519
33	6	0	0.425689	-0.204226	2.706951
34	1	0	0.999153	-1.074766	3.043003
35	1	0	-0.576080	-0.286847	3.133223
36	1	0	0.906634	0.693790	3.108992

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515802	0.000000			
3	H	2.190494	1.092676	0.000000		
4	C	1.406740	2.443437	3.397793	0.000000	
5	C	2.448680	1.567412	2.200665	2.860405	0.000000
6	H	2.705165	2.184450	2.507222	3.263422	1.094197
7	C	2.451275	1.517294	2.185134	2.829058	2.481840
8	C	2.831675	2.449402	3.398072	2.460490	2.899211
9	C	2.473131	2.640056	3.732642	1.536706	2.578474
10	C	2.869447	2.542991	3.495634	2.466782	1.540992
11	H	3.296801	3.320480	4.213334	2.736839	2.206457
12	C	3.624993	2.588889	2.753255	4.142703	3.605554
13	H	3.974551	2.836670	2.559403	4.782903	3.927334
14	C	4.144297	3.753385	4.592919	3.647493	4.185541
15	H	4.802846	4.608054	5.532803	4.017888	4.852766
16	C	4.924529	4.294629	4.883116	4.735075	4.935551
17	H	5.964479	5.380540	5.957657	5.679140	5.972762
18	C	4.719298	3.846270	4.141032	4.936084	4.704762
19	H	5.660885	4.737933	4.854833	5.975400	5.630766
20	C	1.390823	2.588892	2.764566	2.431608	3.566744
21	H	2.152947	2.839300	2.574074	3.416590	3.900111
22	C	2.410390	3.846291	4.152645	2.798993	4.658171
23	H	3.395204	4.739005	4.868521	3.885514	5.585119
24	C	2.781710	4.291566	4.890221	2.416633	4.884927
25	H	3.868323	5.377512	5.965407	3.398509	5.920899
26	C	2.418799	3.747200	4.594370	1.393199	4.138736
27	H	3.409607	4.602648	5.533765	2.159231	4.812514
28	C	3.828079	2.560593	2.836442	4.243901	1.519754
29	C	4.247121	3.542887	4.365661	3.864406	2.415356
30	O	4.614789	3.508807	4.034064	4.634292	2.379563
31	O	5.221085	4.647596	5.519134	4.596805	3.594161
32	O	4.529035	3.130942	2.980203	5.193883	2.452098
33	C	3.827061	4.167739	5.260305	2.567757	3.933020
34	H	4.130925	4.665076	5.738190	2.814954	4.231250
35	H	4.638193	4.679166	5.751306	3.511942	4.253197
36	H	4.149686	4.665626	5.733501	2.845719	4.742970

	6	7	8	9	10

6	H	0.000000				
7	C	3.434113	0.000000			
8	C	3.900491	1.407302	0.000000		
9	C	3.337952	2.466827	1.533657	0.000000	
10	C	2.209230	2.873495	2.483198	1.588397	0.000000
11	H	2.385954	3.884691	3.434833	2.191017	1.094824
12	C	4.523608	1.391753	2.431512	3.775741	4.153585
13	H	4.685988	2.153047	3.416194	4.619458	4.798494
14	C	5.229791	2.421372	1.393519	2.613256	3.622931
15	H	5.858563	3.411139	2.158712	2.871447	3.976308
16	C	6.002508	2.782910	2.415005	3.870747	4.705012
17	H	7.049925	3.869419	3.397230	4.760525	5.636121
18	C	5.712386	2.410196	2.796760	4.323857	4.920327
19	H	6.606185	3.394790	3.883176	5.409679	5.953621
20	C	3.487210	3.623258	4.140523	3.781191	4.149773
21	H	3.711282	3.971162	4.779819	4.625836	4.802083
22	C	4.516001	4.718774	4.932968	4.329698	4.912228
23	H	5.332156	5.659781	5.970852	5.415672	5.947556
24	C	4.867351	4.922612	4.730317	3.874175	4.690279
25	H	5.857647	5.961600	5.672063	4.762621	5.620395
26	C	4.340501	4.140205	3.642334	2.614120	3.604193
27	H	5.073034	4.797725	4.011098	2.871636	3.959594
28	C	2.133324	2.959466	3.488750	3.594205	2.425320
29	C	3.166272	3.450112	2.975310	2.605234	1.525430
30	O	3.099345	3.469692	3.503139	3.563378	2.389458
31	O	4.297898	4.354883	3.589882	3.185796	2.463346
32	O	2.790564	3.563217	4.383729	4.689168	3.600328
33	C	4.605208	3.829169	2.574812	1.527743	2.576108
34	H	4.677210	4.631760	3.515802	2.171078	2.816787
35	H	5.016457	4.154036	2.844834	2.173920	2.822199
36	H	5.438716	4.153712	2.850755	2.172196	3.535446

		11	12	13	14	15
11	H	0.000000				
12	C	5.205772	0.000000			
13	H	5.812070	1.087105	0.000000		
14	C	4.539173	2.805551	3.892620	0.000000	
15	H	4.732571	3.890945	4.977997	1.085478	0.000000
16	C	5.713821	2.420148	3.407518	1.399564	2.154843
17	H	6.611568	3.404533	4.305474	2.153973	2.473703
18	C	5.991792	1.398606	2.162915	2.425467	3.405089
19	H	7.035110	2.155847	2.489551	3.409250	4.300016
20	C	4.387172	4.568491	4.688827	5.377474	6.033023
21	H	5.103575	4.683375	4.547983	6.006763	6.776504
22	C	4.931098	5.714356	5.939705	6.068573	6.545733
23	H	5.923490	6.549549	6.658151	7.083122	7.577420
24	C	4.578551	6.052401	6.502928	5.743162	5.998140
25	H	5.397032	7.070242	7.537802	6.582971	6.722753
26	C	3.543220	5.379555	6.012301	4.610453	4.759465
27	H	3.778279	6.033675	6.780311	4.757412	4.655594
28	C	3.167232	3.638851	3.840826	4.480484	5.192078
29	C	2.131670	4.426909	5.108834	3.680368	3.929604
30	O	3.098963	4.141911	4.595162	4.200436	4.695553

This journal is © The Royal Society of Chemistry 2014

31	O	2.792619	5.252384	6.035178	3.936629	3.878482
32	O	4.298992	3.877762	3.760836	5.297338	6.109502
33	C	2.753223	5.003432	5.953024	3.005965	2.671449
34	H	2.546391	5.900906	6.783937	4.091150	3.749318
35	H	3.083036	5.189124	6.180323	2.943978	2.421321
36	H	3.766364	5.201440	6.191317	2.976291	2.472711

		16	17	18	19	20
16	C	0.000000				
17	H	1.086509	0.000000			
18	C	1.394580	2.153927	0.000000		
19	H	2.154996	2.481964	1.086421	0.000000	
20	C	6.048307	7.066675	5.710797	6.547279	0.000000
21	H	6.492754	7.526991	5.929101	6.647335	1.087534
22	C	6.864974	7.812238	6.714795	7.575825	1.399305
23	H	7.805753	8.741068	7.573160	8.368466	2.157144
24	C	6.731323	7.598561	6.867258	7.811501	2.419248
25	H	7.596308	8.399596	7.813433	8.746363	3.404219
26	C	5.744959	6.587773	6.070806	7.088242	2.803670
27	H	5.998394	6.726303	6.546576	7.581186	3.889145
28	C	4.957302	5.912809	4.603709	5.379268	4.926632
29	C	4.613083	5.399511	4.930011	5.876168	5.572410
30	O	4.775001	5.587149	4.750913	5.549786	5.869163
31	O	4.917270	5.516379	5.495780	6.414332	6.562128
32	O	5.514988	6.445498	4.894402	5.480852	5.446105
33	C	4.405164	5.046227	5.232521	6.296772	4.997260
34	H	5.488171	6.140985	6.255704	7.331115	5.158880
35	H	4.284157	4.795032	5.239112	6.258745	5.901959
36	H	4.316752	4.835113	5.263159	6.285671	5.190512

		21	22	23	24	25
21	H	0.000000				
22	C	2.163173	0.000000			
23	H	2.490278	1.086530	0.000000		
24	C	3.406785	1.394081	2.154999	0.000000	
25	H	4.305353	2.153692	2.482323	1.086621	0.000000
26	C	3.891196	2.425543	3.409800	1.400318	2.154754
27	H	4.976679	3.403998	4.299045	2.153721	2.471691
28	C	5.081533	6.112932	7.009907	6.380465	7.423244
29	C	6.131505	6.410343	7.449144	6.167075	7.075028
30	O	6.199503	6.923589	7.903183	6.938378	7.927279
31	O	7.206320	7.272569	8.334107	6.843960	7.661568
32	O	5.366298	6.738646	7.538573	7.199813	8.263853
33	C	5.949493	5.222341	6.285998	4.390472	5.028139
34	H	6.155373	5.200559	6.219663	4.238920	4.746326
35	H	6.789986	6.248409	7.322953	5.471995	6.118191
36	H	6.181057	5.247314	6.267516	4.297525	4.810883

		26	27	28	29	30
26	C	0.000000				
27	H	1.085554	0.000000			
28	C	5.573361	6.169383	0.000000		
29	C	4.996766	5.194637	2.297106	0.000000	
30	O	5.910621	6.286466	1.388633	1.390020	0.000000
31	O	5.564839	5.538393	3.421648	1.198392	2.253847

This journal is © The Royal Society of Chemistry 2014

32	O	6.531485	7.216463	1.197297	3.425402	2.260262
33	C	2.990370	2.652996	4.800353	3.145947	4.403641
34	H	2.898899	2.374982	5.216213	3.516700	4.845786
35	H	4.073485	3.723628	4.798849	2.816610	4.102594
36	H	2.959469	2.450387	5.656804	4.140237	5.325966

		31	32	33	34	35
31	O	0.000000				
32	O	4.477752	0.000000			
33	C	3.160155	5.958104	0.000000		
34	H	3.481607	6.399968	1.095277	0.000000	
35	H	2.467292	5.952373	1.091822	1.763609	0.000000
36	H	4.124598	6.768154	1.095161	1.772203	1.777829

		36
36	H	0.000000

Stoichiometry C19H14O3
Framework group C1[X(C19H14O3)]
Deg. of freedom 102
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.712680	-0.046539	-0.893769
2	6	0	0.305214	-0.056705	-1.456434
3	1	0	0.276720	-0.000834	-2.547309
4	6	0	1.753103	-0.102166	0.511289
5	6	0	-0.323538	-1.404887	-0.962616
6	1	0	0.217784	-2.239085	-1.419072
7	6	0	-0.468801	1.066857	-0.792588
8	6	0	-0.431095	1.026028	0.613616
9	6	0	0.370938	-0.151602	1.181097
10	6	0	-0.309273	-1.453917	0.577530
11	1	0	0.225396	-2.327098	0.965246
12	6	0	-1.182061	2.062340	-1.453836
13	1	0	-1.213966	2.079635	-2.540335
14	6	0	-1.112047	1.993470	1.349996
15	1	0	-1.100189	1.971660	2.435190
16	6	0	-1.819275	3.000935	0.683946
17	1	0	-2.345529	3.757000	1.260075
18	6	0	-1.855949	3.036120	-0.709708
19	1	0	-2.410482	3.818503	-1.220277
20	6	0	2.887271	-0.005975	-1.637461
21	1	0	2.844512	0.035276	-2.723371
22	6	0	4.121349	-0.011581	-0.977860
23	1	0	5.042496	0.027225	-1.552778
24	6	0	4.167501	-0.064452	0.414453
25	1	0	5.125979	-0.066405	0.926373
26	6	0	2.984708	-0.113117	1.162466
27	1	0	3.037833	-0.153316	2.245974

```
     28          6           0       -1.790467   -1.523535   -1.341687
     29          6           0       -1.779877   -1.604069    0.953982
     30          8           0       -2.563774   -1.633326   -0.193539
     31          8           0       -2.275248   -1.703419    2.040665
     32          8           0       -2.281813   -1.524832   -2.433519
     33          6           0        0.425689   -0.204226    2.706951
     34          1           0        0.999153   -1.074766    3.043003
     35          1           0       -0.576080   -0.286847    3.133223
     36          1           0        0.906634    0.693790    3.108992
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.4273998      0.2799203
0.2691405
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   446 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   446 basis functions,   760 primitive gaussians,   446 cartesian
basis functions
    76 alpha electrons       76 beta electrons
       nuclear repulsion energy      1808.3830094439 Hartrees.
 NAtoms=   36 NActive=   36 NUniq=   36 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   446 RedAO= T  NBF=   446
 NBsUse=   441 1.00D-06 NBFU=   441
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -958.192525361     A.U. after   16 cycles
             Convg  =    0.5869D-08             -V/T =  2.0093


*********************************************************************

            Population analysis using the SCF density.

*********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
```

Supplementary Material (ESI) for Green Chemistry
This journal is © The Royal Society of Chemistry 2014

```
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.23625 -19.17705 -19.17668 -10.35002 -
10.34869
 Alpha  occ. eigenvalues --  -10.24468 -10.24346 -10.24263 -10.23377 -
10.21738
 Alpha  occ. eigenvalues --  -10.21685 -10.21463 -10.21403 -10.21162 -
10.21112
 Alpha  occ. eigenvalues --  -10.21011 -10.20948 -10.20778 -10.20747 -
10.20619
 Alpha  occ. eigenvalues --  -10.20564 -10.19567  -1.15386  -1.08886
-1.04985
 Alpha  occ. eigenvalues --   -0.92467  -0.87027  -0.85215  -0.82348
-0.79405
 Alpha  occ. eigenvalues --   -0.76478  -0.75823  -0.74940  -0.72126
-0.69018
 Alpha  occ. eigenvalues --   -0.67173  -0.64511  -0.61843  -0.61798
-0.60306
 Alpha  occ. eigenvalues --   -0.58064  -0.56350  -0.53879  -0.52805
-0.52118
 Alpha  occ. eigenvalues --   -0.49578  -0.49557  -0.48154  -0.47376
-0.46566
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha  occ. eigenvalues --   -0.45949  -0.45714  -0.45478  -0.44963
-0.44086
 Alpha  occ. eigenvalues --   -0.43566  -0.42924  -0.41780  -0.40833
-0.40118
 Alpha  occ. eigenvalues --   -0.39710  -0.39274  -0.38999  -0.37507
-0.36797
 Alpha  occ. eigenvalues --   -0.35910  -0.35772  -0.34404  -0.34158
-0.33998
 Alpha  occ. eigenvalues --   -0.31642  -0.29190  -0.27099  -0.26963
-0.26584
 Alpha  occ. eigenvalues --   -0.25211
 Alpha virt. eigenvalues --   -0.04617  -0.03694  -0.03513  -0.03098
-0.01312
 Alpha virt. eigenvalues --   -0.01217  -0.00652   0.00333   0.00635
 0.00741
 Alpha virt. eigenvalues --    0.02302   0.02468   0.03376   0.03593
 0.03984
 Alpha virt. eigenvalues --    0.04670   0.04837   0.05500   0.05928
 0.06433
 Alpha virt. eigenvalues --    0.06845   0.06906   0.07833   0.08309
 0.08432
 Alpha virt. eigenvalues --    0.08900   0.09527   0.10048   0.10249
 0.10503
 Alpha virt. eigenvalues --    0.11112   0.11336   0.12012   0.12264
 0.12707
 Alpha virt. eigenvalues --    0.12924   0.13214   0.13471   0.13818
 0.14002
 Alpha virt. eigenvalues --    0.14171   0.14909   0.15292   0.15620
 0.15781
 Alpha virt. eigenvalues --    0.15939   0.16209   0.16501   0.16716
 0.17132
 Alpha virt. eigenvalues --    0.17289   0.17645   0.17939   0.18490
 0.18881
 Alpha virt. eigenvalues --    0.19157   0.19407   0.19986   0.20254
 0.20392
 Alpha virt. eigenvalues --    0.20550   0.20755   0.21120   0.21472
 0.21804
 Alpha virt. eigenvalues --    0.21864   0.22321   0.22501   0.22765
 0.23136
 Alpha virt. eigenvalues --    0.23476   0.23673   0.24142   0.24363
 0.24756
 Alpha virt. eigenvalues --    0.24953   0.25582   0.25610   0.26222
 0.26295
 Alpha virt. eigenvalues --    0.26444   0.27141   0.27656   0.27852
 0.28096
 Alpha virt. eigenvalues --    0.28416   0.28723   0.28870   0.29607
 0.29723
 Alpha virt. eigenvalues --    0.29858   0.30529   0.30978   0.31154
 0.31503
 Alpha virt. eigenvalues --    0.32174   0.32552   0.32596   0.33142
 0.33255
```

```
 Alpha virt. eigenvalues --    0.34009   0.34748   0.34961   0.35238
0.35933
 Alpha virt. eigenvalues --    0.36211   0.36693   0.37351   0.38161
0.38976
 Alpha virt. eigenvalues --    0.39291   0.39636   0.40460   0.41436
0.41602
 Alpha virt. eigenvalues --    0.42052   0.42456   0.43060   0.43454
0.44237
 Alpha virt. eigenvalues --    0.45556   0.46406   0.47483   0.49077
0.51273
 Alpha virt. eigenvalues --    0.52390   0.56297   0.57700   0.58790
0.60281
 Alpha virt. eigenvalues --    0.62068   0.64929   0.67279   0.68134
0.68927
 Alpha virt. eigenvalues --    0.69657   0.70824   0.71316   0.71519
0.72091
 Alpha virt. eigenvalues --    0.72628   0.73054   0.73470   0.73953
0.75058
 Alpha virt. eigenvalues --    0.75483   0.76628   0.76837   0.77143
0.77859
 Alpha virt. eigenvalues --    0.78794   0.79168   0.79776   0.80776
0.81227
 Alpha virt. eigenvalues --    0.81659   0.81718   0.82814   0.83479
0.84545
 Alpha virt. eigenvalues --    0.85152   0.85852   0.87149   0.87334
0.88601
 Alpha virt. eigenvalues --    0.89194   0.89272   0.90638   0.91140
0.92503
 Alpha virt. eigenvalues --    0.93836   0.93999   0.94473   0.96103
0.97300
 Alpha virt. eigenvalues --    0.97600   0.99174   0.99865   1.00446
1.00706
 Alpha virt. eigenvalues --    1.02138   1.02677   1.03409   1.05051
1.05397
 Alpha virt. eigenvalues --    1.06088   1.06794   1.08790   1.09815
1.10271
 Alpha virt. eigenvalues --    1.12141   1.14429   1.14780   1.15443
1.16408
 Alpha virt. eigenvalues --    1.17562   1.18368   1.18897   1.19743
1.21811
 Alpha virt. eigenvalues --    1.22627   1.23400   1.24295   1.25675
1.26418
 Alpha virt. eigenvalues --    1.27242   1.28456   1.30577   1.32120
1.33111
 Alpha virt. eigenvalues --    1.33660   1.35006   1.35920   1.36466
1.36981
 Alpha virt. eigenvalues --    1.37466   1.39340   1.39835   1.40360
1.41560
 Alpha virt. eigenvalues --    1.43450   1.43838   1.43996   1.44623
1.45410
 Alpha virt. eigenvalues --    1.46277   1.47151   1.48703   1.49059
1.49596
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    1.50490   1.51001   1.53973   1.55580
1.57919
 Alpha virt. eigenvalues --    1.58678   1.61344   1.63002   1.65003
1.68248
 Alpha virt. eigenvalues --    1.70844   1.70948   1.71588   1.74158
1.76867
 Alpha virt. eigenvalues --    1.78279   1.78409   1.79168   1.80975
1.81967
 Alpha virt. eigenvalues --    1.82889   1.83446   1.83785   1.85331
1.86912
 Alpha virt. eigenvalues --    1.87831   1.88425   1.89130   1.90110
1.90761
 Alpha virt. eigenvalues --    1.91381   1.92669   1.94494   1.96080
1.96876
 Alpha virt. eigenvalues --    1.97490   1.98292   1.99119   2.01142
2.01719
 Alpha virt. eigenvalues --    2.02112   2.02905   2.04003   2.05382
2.07583
 Alpha virt. eigenvalues --    2.07786   2.08895   2.10012   2.12552
2.13625
 Alpha virt. eigenvalues --    2.14584   2.17241   2.18202   2.18599
2.19739
 Alpha virt. eigenvalues --    2.21225   2.22369   2.24202   2.25290
2.26958
 Alpha virt. eigenvalues --    2.28204   2.29408   2.29790   2.31324
2.31937
 Alpha virt. eigenvalues --    2.33915   2.34049   2.37067   2.37610
2.39148
 Alpha virt. eigenvalues --    2.40954   2.43366   2.43949   2.46080
2.50189
 Alpha virt. eigenvalues --    2.51534   2.53399   2.54976   2.58944
2.59928
 Alpha virt. eigenvalues --    2.60907   2.64281   2.65959   2.67247
2.69682
 Alpha virt. eigenvalues --    2.69833   2.71358   2.72044   2.73219
2.75663
 Alpha virt. eigenvalues --    2.76399   2.78600   2.79678   2.80659
2.83110
 Alpha virt. eigenvalues --    2.84220   2.85426   2.85832   2.86717
2.88001
 Alpha virt. eigenvalues --    2.90824   2.94998   2.96772   3.05614
3.09479
 Alpha virt. eigenvalues --    3.11117   3.13501   3.23456   3.23792
3.27368
 Alpha virt. eigenvalues --    3.33883   3.41432   3.41797   4.24080
4.25672
 Alpha virt. eigenvalues --    4.27861   4.31214   4.32860   4.34454
4.36341
 Alpha virt. eigenvalues --    4.39563   4.41921   4.45194   4.48572
4.49237
 Alpha virt. eigenvalues --    4.50919   4.52821   4.60393   4.67523
4.73263
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    4.76010   4.80826   4.85311   5.15793
5.37804
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   14.609732  -3.815198  -0.051103   1.883715  -0.109583
0.043054
     2  C   -3.815198  17.380423   0.265997  -4.953831  -1.600115  -
0.052844
     3  H   -0.051103   0.265997   0.532181  -0.010253  -0.001822  -
0.002994
     4  C    1.883715  -4.953831  -0.010253  25.224109   1.606981
0.021853
     5  C   -0.109583  -1.600115  -0.001822   1.606981  10.906555
0.349474
     6  H    0.043054  -0.052844  -0.002994   0.021853   0.349474
0.481106
     7  C   -0.086318  -4.606980  -0.060868   0.306884   0.659669
0.030021
     8  C    3.936506  -6.699777   0.004322  -0.070030   1.117450
0.016496
     9  C   -2.878151   4.734277  -0.009351  -1.849575  -1.692841  -
0.019441
    10  C    0.375088  -0.436743   0.026034  -0.928807  -2.986127  -
0.023246
    11  H   -0.049574  -0.010944  -0.000126   0.108514  -0.011241  -
0.004621
    12  C   -0.677863   2.151625   0.035480  -0.647481  -0.403704
0.008787
    13  H   -0.022134  -0.024215   0.003340  -0.004342  -0.012731  -
0.000007
    14  C   -2.594271   2.122229   0.001047   0.660438  -0.509211
0.001905
    15  H    0.000808   0.009455   0.000002  -0.000674   0.001231
0.000000
    16  C   -0.005118  -0.320254   0.003179   0.244758  -0.030707
0.000267
    17  H    0.002469   0.001767   0.000000  -0.003345   0.001088
0.000000
    18  C   -0.305715  -0.028521   0.007091  -0.048010  -0.053599
0.001043
    19  H   -0.003283  -0.016788  -0.000004   0.001853  -0.000499
0.000000
    20  C   -1.046531   0.167867   0.036992  -3.835940   0.524582  -
0.029184
    21  H   -0.021287  -0.046124   0.003373   0.062001   0.010287  -
0.000061
    22  C   -0.733123  -0.492901   0.002225  -0.824912   0.073643  -
0.004518
    23  H    0.007142  -0.014291  -0.000004   0.022158  -0.001276
0.000001
    24  C   -0.268120   0.075398  -0.000218   1.901584  -0.091065
0.005051
```

This journal is © The Royal Society of Chemistry 2014

25	H	0.001092	0.001756	0.000000	0.034489	0.000744	0.000000
26	C	1.413555	0.272729	0.013044	-11.076352	-0.127006	-0.005056
27	H	0.032396	-0.001582	0.000003	-0.152228	-0.002515	0.000000
28	C	-0.591926	0.527415	-0.017137	-0.442112	-1.230830	-0.080743
29	C	-0.302625	0.577928	-0.001309	-0.368105	0.507730	0.004874
30	O	-0.000627	0.133215	-0.000469	-0.003977	-0.351524	0.005422
31	O	0.022750	-0.048786	0.000074	-0.011273	-0.026496	-0.000665
32	O	0.007705	-0.076421	0.005216	0.011825	-0.024670	-0.002027
33	C	-2.202829	0.409513	0.005018	-0.967007	-0.202665	0.004803
34	H	-0.012529	0.000336	0.000000	-0.031911	0.008858	-0.000001
35	H	0.007139	-0.010656	0.000000	0.063446	0.002926	0.000002
36	H	-0.028774	0.007623	0.000000	-0.073091	-0.007750	0.000002

		7	8	9	10	11	12
1	C	-0.086318	3.936506	-2.878151	0.375088	-0.049574	-0.677863
2	C	-4.606980	-6.699777	4.734277	-0.436743	-0.010944	2.151625
3	H	-0.060868	0.004322	-0.009351	0.026034	-0.000126	0.035480
4	C	0.306884	-0.070030	-1.849575	-0.928807	0.108514	-0.647481
5	C	0.659669	1.117450	-1.692841	-2.986127	-0.011241	-0.403704
6	H	0.030021	0.016496	-0.019441	-0.023246	-0.004621	0.008787
7	C	18.263813	7.113323	-3.788000	-0.267208	-0.002971	-6.280160
8	C	7.113323	37.104389	-2.987029	-2.339959	-0.014894	-7.646347
9	C	-3.788000	-2.987029	17.874918	-0.404975	-0.045178	1.045176
10	C	-0.267208	-2.339959	-0.404975	11.820920	0.354503	0.338084
11	H	-0.002971	-0.014894	-0.045178	0.354503	0.480132	-0.003200
12	C	-6.280160	-7.646347	1.045176	0.338084	-0.003200	11.665932
13	H	-0.073404	0.047022	0.020315	0.001110	0.000000	0.292346

```
    14  C   -4.140187 -19.290643   0.579205   1.139683   0.023347
5.559385
    15  H    0.039808  -0.196879   0.000371  -0.014490  -0.000004  -
0.009753
    16  C    0.647802   0.175286  -0.037202  -0.005742   0.001360  -
1.234380
    17  H    0.017416   0.044911  -0.015127  -0.001306   0.000000
0.009523
    18  C   -1.780491  -1.031447   0.211297   0.051619  -0.000139
1.342087
    19  H    0.016868   0.037962   0.001682   0.000624   0.000000  -
0.003274
    20  C    1.311557   0.361911  -1.594278  -0.402572  -0.013633  -
0.783895
    21  H    0.003082   0.004702   0.003713  -0.002804   0.000000
0.001276
    22  C    0.088529   0.314516  -0.324029  -0.059448  -0.005270  -
0.249489
    23  H   -0.003452   0.000515   0.001431   0.000897   0.000000
0.000364
    24  C   -0.128995  -0.762201   0.088104   0.335766   0.009088
0.190270
    25  H    0.000449  -0.004401  -0.012856  -0.000704   0.000001  -
0.000158
    26  C    0.638183   2.561118  -1.038528  -0.452977  -0.048522  -
0.642135
    27  H    0.008916   0.026006   0.017220   0.002935  -0.000073
0.002033
    28  C   -0.869619  -0.793955   0.853042   0.584593   0.014151
0.472642
    29  C   -0.169230  -0.358831  -0.061923  -0.884409  -0.075869
0.233087
    30  O   -0.117152  -0.124865   0.104641  -0.201602   0.005319
0.015054
    31  O    0.031216   0.257813  -0.049420  -0.171314  -0.002047  -
0.011129
    32  O    0.129470   0.046905  -0.043874  -0.067336  -0.000641  -
0.091676
    33  C   -0.525403  -4.789470  -1.944852   0.634011   0.035346
1.001506
    34  H    0.003556   0.035682  -0.055238  -0.069549   0.003425
0.001486
    35  H    0.000345  -0.071025  -0.031756  -0.017361   0.000056
0.000956
    36  H    0.005425  -0.150777  -0.061475   0.054026   0.000080
0.006580
              13         14         15         16         17         18
     1  C   -0.022134  -2.594271   0.000808  -0.005118   0.002469  -
0.305715
     2  C   -0.024215   2.122229   0.009455  -0.320254   0.001767  -
0.028521
```

This journal is © The Royal Society of Chemistry 2014

3	H	0.003340	0.001047	0.000002	0.003179	0.000000	0.007091
4	C	-0.004342	0.660438	-0.000674	0.244758	-0.003345	-0.048010
5	C	-0.012731	-0.509211	0.001231	-0.030707	0.001088	-0.053599
6	H	-0.000007	0.001905	0.000000	0.000267	0.000000	0.001043
7	C	-0.073404	-4.140187	0.039808	0.647802	0.017416	-1.780491
8	C	0.047022	-19.290643	-0.196879	0.175286	0.044911	-1.031447
9	C	0.020315	0.579205	0.000371	-0.037202	-0.015127	0.211297
10	C	0.001110	1.139683	-0.014490	-0.005742	-0.001306	0.051619
11	H	0.000000	0.023347	-0.000004	0.001360	0.000000	-0.000139
12	C	0.292346	5.559385	-0.009753	-1.234380	0.009523	1.342087
13	H	0.535498	-0.015135	0.000019	0.007346	-0.000163	0.050682
14	C	-0.015135	21.078815	0.344985	-0.692455	0.015491	0.501618
15	H	0.000019	0.344985	0.537955	0.077493	-0.004474	0.016358
16	C	0.007346	-0.692455	0.077493	6.807050	0.286059	0.605380
17	H	-0.000163	0.015491	-0.004474	0.286059	0.529003	-0.061903
18	C	0.050682	0.501618	0.016358	0.605380	-0.061903	6.501403
19	H	-0.004240	-0.001844	-0.000163	-0.042604	-0.004246	0.305010
20	C	-0.004516	-0.781242	0.001558	0.016892	-0.000075	-0.113877
21	H	0.000000	0.000267	0.000000	-0.000043	0.000000	0.000585
22	C	-0.000604	-0.244448	-0.000011	0.008279	0.000027	-0.037501
23	H	0.000000	-0.000151	0.000000	-0.000009	0.000000	-0.000003
24	C	-0.000012	0.434359	-0.001673	-0.034113	-0.000027	0.027266
25	H	0.000000	0.000748	0.000000	0.000008	0.000000	0.000002
26	C	0.000055	-2.343468	-0.006327	-0.088557	0.000644	-0.074596
27	H	0.000000	-0.005997	0.000000	-0.001506	0.000000	0.000083
28	C	0.016234	0.704584	-0.000937	-0.019197	-0.001235	0.016796

This journal is © The Royal Society of Chemistry 2014

29	C	-0.000955	0.099180	0.017822	-0.006447	0.001582
0.035849						
30	O	-0.000116	0.029739	-0.000120	-0.008865	-0.000005
0.006309						
31	O	-0.000002	-0.144034	-0.000760	-0.010150	-0.000039
-0.005969						
32	O	-0.000212	-0.035820	-0.000002	0.002254	0.000003
-0.014638						
33	C	0.002045	3.597184	0.001377	0.009999	-0.001877
0.143865						
34	H	0.000000	0.000851	0.000081	-0.001861	0.000000
0.000285						
35	H	0.000000	0.027477	-0.000858	0.007138	-0.000001
0.000055						
36	H	0.000000	0.076728	-0.000632	-0.003342	0.000000
0.001044						

		19	20	21	22	23	24
1	C	-0.003283	-1.046531	-0.021287	-0.733123	0.007142	
-0.268120							
2	C	-0.016788	0.167867	-0.046124	-0.492901	-0.014291	
0.075398							
3	H	-0.000004	0.036992	0.003373	0.002225	-0.000004	
-0.000218							
4	C	0.001853	-3.835940	0.062001	-0.824912	0.022158	
1.901584							
5	C	-0.000499	0.524582	0.010287	0.073643	-0.001276	
-0.091065							
6	H	0.000000	-0.029184	-0.000061	-0.004518	0.000001	
0.005051							
7	C	0.016868	1.311557	0.003082	0.088529	-0.003452	
-0.128995							
8	C	0.037962	0.361911	0.004702	0.314516	0.000515	
-0.762201							
9	C	0.001682	-1.594278	0.003713	-0.324029	0.001431	
0.088104							
10	C	0.000624	-0.402572	-0.002804	-0.059448	0.000897	
0.335766							
11	H	0.000000	-0.013633	0.000000	-0.005270	0.000000	
0.009088							
12	C	-0.003274	-0.783895	0.001276	-0.249489	0.000364	
0.190270							
13	H	-0.004240	-0.004516	0.000000	-0.000604	0.000000	
-0.000012							
14	C	-0.001844	-0.781242	0.000267	-0.244448	-0.000151	
0.434359							
15	H	-0.000163	0.001558	0.000000	-0.000011	0.000000	
-0.001673							
16	C	-0.042604	0.016892	-0.000043	0.008279	-0.000009	
-0.034113							
17	H	-0.004246	-0.000075	0.000000	0.000027	0.000000	
-0.000027							

This journal is © The Royal Society of Chemistry 2014

```
    18  C    0.305010  -0.113877   0.000585  -0.037501  -0.000003
0.027266
    19  H    0.527570   0.000326   0.000000  -0.000002   0.000000  -
0.000001
    20  C    0.000326   9.750700   0.263377   0.807935  -0.003836  -
1.306246
    21  H    0.000000   0.263377   0.538776   0.014073  -0.004238
0.012161
    22  C   -0.000002   0.807935   0.014073   6.803611   0.307373
0.478880
    23  H    0.000000  -0.003836  -0.004238   0.307373   0.528369  -
0.029203
    24  C   -0.000001  -1.306246   0.012161   0.478880  -0.029203
7.502851
    25  H    0.000000   0.021483  -0.000163  -0.042136  -0.004259
0.302139
    26  C   -0.000232   2.985135  -0.027722   0.628781   0.007952  -
3.051085
    27  H    0.000000  -0.018203   0.000019   0.023608  -0.000162
0.054152
    28  C    0.001412  -0.270766   0.002418  -0.025712  -0.000015
0.031061
    29  C   -0.001121   0.017645  -0.000569  -0.018870  -0.000064
0.031679
    30  O   -0.000012   0.017671   0.000000   0.002356   0.000000  -
0.001348
    31  O    0.000004   0.002415   0.000000   0.000267   0.000000  -
0.002568
    32  O   -0.000035   0.022415   0.000002   0.000387   0.000000  -
0.000622
    33  C   -0.000013  -0.273076   0.000795  -0.219484   0.000374
0.469455
    34  H    0.000000  -0.002510   0.000000  -0.000770   0.000000
0.014758
    35  H    0.000000   0.001175   0.000000   0.000175   0.000000  -
0.001770
    36  H    0.000000  -0.001925   0.000000  -0.000692   0.000000
0.010665
              25         26         27         28         29         30
     1  C    0.001092   1.413555   0.032396  -0.591926  -0.302625  -
0.000627
     2  C    0.001756   0.272729  -0.001582   0.527415   0.577928
0.133215
     3  H    0.000000   0.013044   0.000003  -0.017137  -0.001309  -
0.000469
     4  C    0.034489 -11.076352  -0.152228  -0.442112  -0.368105  -
0.003977
     5  C    0.000744  -0.127006  -0.002515  -1.230830   0.507730  -
0.351524
     6  H    0.000000  -0.005056   0.000000  -0.080743   0.004874
0.005422
```

This journal is © The Royal Society of Chemistry 2014

```
     7  C    0.000449   0.638183   0.008916  -0.869619  -0.169230  -
0.117152
     8  C   -0.004401   2.561118   0.026006  -0.793955  -0.358831  -
0.124865
     9  C   -0.012856  -1.038528   0.017220   0.853042  -0.061923
0.104641
    10  C   -0.000704  -0.452977   0.002935   0.584593  -0.884409  -
0.201602
    11  H    0.000001  -0.048522  -0.000073   0.014151  -0.075869
0.005319
    12  C   -0.000158  -0.642135   0.002033   0.472642   0.233087
0.015054
    13  H    0.000000   0.000055   0.000000   0.016234  -0.000955  -
0.000116
    14  C    0.000748  -2.343468  -0.005997   0.704584   0.099180
0.029739
    15  H    0.000000  -0.006327   0.000000  -0.000937   0.017822  -
0.000120
    16  C    0.000008  -0.088557  -0.001506  -0.019197  -0.006447  -
0.008865
    17  H    0.000000   0.000644   0.000000  -0.001235   0.001582  -
0.000005
    18  C    0.000002  -0.074596   0.000083   0.016796   0.035849
0.006309
    19  H    0.000000  -0.000232   0.000000   0.001412  -0.001121  -
0.000012
    20  C    0.021483   2.985135  -0.018203  -0.270766   0.017645
0.017671
    21  H   -0.000163  -0.027722   0.000019   0.002418  -0.000569
0.000000
    22  C   -0.042136   0.628781   0.023608  -0.025712  -0.018870
0.002356
    23  H   -0.004259   0.007952  -0.000162  -0.000015  -0.000064
0.000000
    24  C    0.302139  -3.051085   0.054152   0.031061   0.031679  -
0.001348
    25  H    0.530147  -0.006212  -0.004491  -0.000084   0.000041
0.000000
    26  C   -0.006212  17.930566   0.313580  -0.180155   0.038758
0.017332
    27  H   -0.004491   0.313580   0.538942  -0.000244   0.002097  -
0.000003
    28  C   -0.000084  -0.180155  -0.000244   6.642327  -0.761625
0.285265
    29  C    0.000041   0.038758   0.002097  -0.761625   6.276359
0.217392
    30  O    0.000000   0.017332  -0.000003   0.285265   0.217392
8.362594
    31  O    0.000000   0.001994   0.000012   0.027275   0.483853  -
0.069614
    32  O    0.000000   0.003920   0.000000   0.440421   0.043921  -
0.083612
```

This journal is © The Royal Society of Chemistry 2014

33	C	-0.000422	-1.364825	-0.019262	0.337150	0.152245	-0.004349
34	H	0.000000	0.000833	-0.000959	0.000770	0.001752	-0.000183
35	H	0.000000	-0.010650	0.000078	-0.005130	0.010226	0.000073
36	H	0.000001	-0.011825	-0.000569	0.002378	-0.001145	0.000020

		31	32	33	34	35	36
1	C	0.022750	0.007705	-2.202829	-0.012529	0.007139	-0.028774
2	C	-0.048786	-0.076421	0.409513	0.000336	-0.010656	0.007623
3	H	0.000074	0.005216	0.005018	0.000000	0.000000	0.000000
4	C	-0.011273	0.011825	-0.967007	-0.031911	0.063446	-0.073091
5	C	-0.026496	-0.024670	-0.202665	0.008858	0.002926	-0.007750
6	H	-0.000665	-0.002027	0.004803	-0.000001	0.000002	0.000002
7	C	0.031216	0.129470	-0.525403	0.003556	0.000345	0.005425
8	C	0.257813	0.046905	-4.789470	0.035682	-0.071025	-0.150777
9	C	-0.049420	-0.043874	-1.944852	-0.055238	-0.031756	-0.061475
10	C	-0.171314	-0.067336	0.634011	-0.069549	-0.017361	0.054026
11	H	-0.002047	-0.000641	0.035346	0.003425	0.000056	0.000080
12	C	-0.011129	-0.091676	1.001506	0.001486	0.000956	0.006580
13	H	-0.000002	-0.000212	0.002045	0.000000	0.000000	0.000000
14	C	-0.144034	-0.035820	3.597184	0.000851	0.027477	0.076728
15	H	-0.000760	-0.000002	0.001377	0.000081	-0.000858	-0.000632
16	C	-0.010150	0.002254	0.009999	-0.001861	0.007138	-0.003342
17	H	-0.000039	0.000003	-0.001877	0.000000	-0.000001	0.000000
18	C	-0.005969	-0.014638	0.143865	0.000285	0.000055	0.001044
19	H	0.000004	-0.000035	-0.000013	0.000000	0.000000	0.000000
20	C	0.002415	0.022415	-0.273076	-0.002510	0.001175	-0.001925
21	H	0.000000	0.000002	0.000795	0.000000	0.000000	0.000000

This journal is © The Royal Society of Chemistry 2014

```
    22  C    0.000267   0.000387  -0.219484  -0.000770   0.000175  -
0.000692
    23  H    0.000000   0.000000   0.000374   0.000000   0.000000
0.000000
    24  C   -0.002568  -0.000622   0.469455   0.014758  -0.001770
0.010665
    25  H    0.000000   0.000000  -0.000422   0.000000   0.000000
0.000001
    26  C    0.001994   0.003920  -1.364825   0.000833  -0.010650  -
0.011825
    27  H    0.000012   0.000000  -0.019262  -0.000959   0.000078  -
0.000569
    28  C    0.027275   0.440421   0.337150   0.000770  -0.005130
0.002378
    29  C    0.483853   0.043921   0.152245   0.001752   0.010226  -
0.001145
    30  O   -0.069614  -0.083612  -0.004349  -0.000183   0.000073
0.000020
    31  O    8.141090  -0.000014  -0.035257   0.000790  -0.010188
0.000692
    32  O   -0.000014   8.111369  -0.005318  -0.000001   0.000011  -
0.000003
    33  C   -0.035257  -0.005318  10.694360   0.425557   0.370926
0.497711
    34  H    0.000790  -0.000001   0.425557   0.498728  -0.024583  -
0.028303
    35  H   -0.010188   0.000011   0.370926  -0.024583   0.443663  -
0.026156
    36  H    0.000692  -0.000003   0.497711  -0.028303  -0.026156
0.493944
 Mulliken atomic charges:
              1
     1  C   -0.536468
     2  C    0.417419
     3  H    0.211037
     4  C    0.148647
     5  C   -0.293239
     6  H    0.251245
     7  C   -0.415895
     8  C    0.125695
     9  C   -0.590294
    10  C    0.018786
    11  H    0.253626
    12  C    0.310964
    13  H    0.186775
    14  C   -0.200359
    15  H    0.188434
    16  C   -0.357997
    17  H    0.183841
    18  C   -0.269316
    19  H    0.185049
    20  C    0.170668
```

```
    21  H    0.182104
    22  C   -0.270746
    23  H    0.184388
    24  C   -0.295421
    25  H    0.182787
    26  C   -0.271950
    27  H    0.185714
    28  C    0.331488
    29  C    0.259078
    30  O   -0.233961
    31  O   -0.370520
    32  O   -0.378901
    33  C   -0.237130
    34  H    0.230648
    35  H    0.274265
    36  H    0.239539
 Sum of Mulliken atomic charges =   0.00000
 Mulliken charges with hydrogens summed into heavy atoms:
              1
     1  C   -0.536468
     2  C    0.628457
     4  C    0.148647
     5  C   -0.041994
     7  C   -0.415895
     8  C    0.125695
     9  C   -0.590294
    10  C    0.272412
    12  C    0.497739
    14  C   -0.011926
    16  C   -0.174156
    18  C   -0.084267
    20  C    0.352773
    22  C   -0.086358
    24  C   -0.112635
    26  C   -0.086236
    28  C    0.331488
    29  C    0.259078
    30  O   -0.233961
    31  O   -0.370520
    32  O   -0.378901
    33  C    0.507323
 Sum of Mulliken charges with hydrogens summed into heavy atoms =
0.00000
 Electronic spatial extent (au):  <R**2>=           4995.0759
 Charge=              0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=              4.7265    Y=              1.2102    Z=
0.3094  Tot=              4.8888
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=           -135.6126   YY=           -125.0620   ZZ=           -
127.6536
```

```
   XY=            -12.2850   XZ=             -1.1786   YZ=
-0.0084
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=             -6.1699   YY=              4.3807   ZZ=
1.7891
   XY=            -12.2850   XZ=             -1.1786   YZ=
-0.0084
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=             57.5863  YYY=            -17.8820  ZZZ=
4.6136  XYY=           -26.9627
  XXY=             27.7676  XXZ=              1.9812  XZZ=
32.4634  YZZ=            23.2283
  YYZ=             -1.3224  XYZ=             -0.3494
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=          -3311.7259 YYYY=          -1727.7647 ZZZZ=          -
1643.4345 XXXY=           -38.8304
 XXXZ=            -13.0463 YYYX=            -48.1798 YYYZ=
8.3971 ZZZX=           -26.4886
 ZZZY=            -11.4625 XXYY=           -907.4490 XXZZ=           -
868.2477 YYZZ=           -581.7964
 XXYZ=             -5.8204 YYXZ=             10.7106 ZZXY=
-61.5417
 N-N= 1.808383009444D+03 E-N=-5.842121900867D+03  KE=
9.493403123251D+02
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6          -0.001213894   -0.000279109    0.000225921
      2          6          -0.000004789    0.000361142   -0.000203961
      3          1           0.000222108    0.000199297   -0.000159124
      4          6          -0.001168809   -0.000191390   -0.000149039
      5          6          -0.000417498   -0.000095449   -0.000230977
      6          1           0.000013244   -0.000239634   -0.000217341
      7          6           0.000637067   -0.000686481    0.000099868
      8          6           0.000541833   -0.000580072   -0.000179829
      9          6           0.000071771    0.000337062    0.000338203
     10          6          -0.000382388   -0.000259102    0.000305430
     11          1           0.000071160   -0.000236993    0.000153326
     12          6           0.000291778    0.000002161   -0.001076123
     13          1          -0.000101868    0.000025308   -0.000354183
     14          6           0.000360798   -0.000121161    0.000972213
     15          1          -0.000150891    0.000048228    0.000279838
     16          6          -0.000567962    0.000905350    0.000899227
     17          1          -0.000166497    0.000169869    0.000135589
     18          6          -0.000568339    0.000981589   -0.000791152
     19          1          -0.000169447    0.000177406   -0.000104045
     20          6          -0.000368946    0.000091326   -0.001257084
     21          1           0.000076266    0.000032855   -0.000355301
```

```
     22        6           0.001249304    0.000041541   -0.000791309
     23        1           0.000228741    0.000018720   -0.000110129
     24        6           0.001303221    0.000027624    0.000725332
     25        1           0.000239625    0.000006482    0.000106306
     26        6          -0.000296542   -0.000068298    0.001137797
     27        1           0.000181121    0.000011688    0.000228400
     28        6           0.001990597    0.000336038    0.002291008
     29        6           0.001506648    0.000360062   -0.000892709
     30        8          -0.000884471   -0.000250078   -0.000612316
     31        8          -0.001135850   -0.000739458    0.001412118
     32        8          -0.001587748   -0.000530716   -0.002411627
     33        6           0.000204442    0.000033712   -0.000352683
     34        1          -0.000062893   -0.000288908    0.000228720
     35        1          -0.000015922    0.000181174    0.000472183
     36        1           0.000075030    0.000218217    0.000237455
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.002411627 RMS     0.000660753


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.002847691 RMS     0.000449296
 Search for a local minimum.
 Step number   1 out of a maximum of  216
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Second derivative matrix not updated -- first step.
     Eigenvalues ---    0.00399   0.00430   0.00694   0.00788
0.01147
     Eigenvalues ---    0.01164   0.01214   0.01430   0.01482
0.01563
     Eigenvalues ---    0.01785   0.02112   0.02117   0.02127
0.02130
     Eigenvalues ---    0.02131   0.02133   0.02141   0.02142
0.02155
     Eigenvalues ---    0.02157   0.02162   0.02166   0.02806
0.03427
     Eigenvalues ---    0.04146   0.04613   0.05002   0.05217
0.05318
     Eigenvalues ---    0.05360   0.05536   0.05619   0.05769
0.06535
     Eigenvalues ---    0.08069   0.08564   0.09328   0.10022
0.12593
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16380   0.20243   0.21664
0.22000
     Eigenvalues ---    0.22000   0.22343   0.22611   0.22631
0.24428
```

Eigenvalues --- 0.24583 0.24594 0.24998 0.25000
0.26104
Eigenvalues --- 0.27449 0.27685 0.28709 0.28943
0.29633
Eigenvalues --- 0.29818 0.30070 0.34210 0.34223
0.34261
Eigenvalues --- 0.34332 0.34505 0.34603 0.35099
0.35149
Eigenvalues --- 0.35206 0.35217 0.35219 0.35230
0.35332
Eigenvalues --- 0.35340 0.36674 0.39929 0.41993
0.42036
Eigenvalues --- 0.43454 0.44130 0.44491 0.46015
0.46044
Eigenvalues --- 0.46071 0.46353 0.46360 0.46795
0.46911
Eigenvalues --- 1.05635
1.061931000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-2.33030442D-04 EMin= 3.98966307D-03
 Linear search not attempted -- first point.
 Iteration  1 RMS(Cart)=  0.01380637 RMS(Int)=  0.00014854
 Iteration  2 RMS(Cart)=  0.00014680 RMS(Int)=  0.00004939
 Iteration  3 RMS(Cart)=  0.00000004 RMS(Int)=  0.00004939
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.86445  -0.00005   0.00000  -0.00043  -0.00044
2.86401
    R2        2.65835   0.00066   0.00000   0.00188   0.00186
2.66022
    R3        2.62827   0.00156   0.00000   0.00325   0.00325
2.63152
    R4        2.06486   0.00016   0.00000   0.00047   0.00047
2.06533
    R5        2.96198   0.00080   0.00000   0.00296   0.00296
2.96494
    R6        2.86727   0.00028   0.00000   0.00069   0.00069
2.86796
    R7        2.90395   0.00027   0.00000   0.00182   0.00181
2.90577
    R8        2.63276   0.00156   0.00000   0.00330   0.00330
2.63607
    R9        2.06773   0.00028   0.00000   0.00082   0.00082
2.06855
   R10        2.91205   0.00103   0.00000   0.00259   0.00260
2.91466
   R11        2.87192   0.00001   0.00000  -0.00035  -0.00036
2.87155
   R12        2.65942   0.00089   0.00000   0.00165   0.00166
2.66107
```

This journal is © The Royal Society of Chemistry 2014

R13	2.63003	0.00143	0.00000	0.00303	0.00303
2.63306					
R14	2.89819	0.00060	0.00000	0.00186	0.00186
2.90005					
R15	2.63337	0.00139	0.00000	0.00296	0.00296
2.63633					
R16	3.00163	0.00118	0.00000	0.00472	0.00472
3.00636					
R17	2.88702	0.00059	0.00000	0.00199	0.00199
2.88900					
R18	2.06892	0.00028	0.00000	0.00082	0.00082
2.06973					
R19	2.88265	0.00028	0.00000	0.00095	0.00097
2.88362					
R20	2.05433	0.00036	0.00000	0.00102	0.00102
2.05535					
R21	2.64298	0.00146	0.00000	0.00319	0.00319
2.64617					
R22	2.05126	0.00027	0.00000	0.00078	0.00078
2.05203					
R23	2.64479	0.00147	0.00000	0.00321	0.00321
2.64800					
R24	2.05320	0.00027	0.00000	0.00076	0.00076
2.05397					
R25	2.63537	0.00157	0.00000	0.00339	0.00339
2.63877					
R26	2.05304	0.00026	0.00000	0.00075	0.00075
2.05379					
R27	2.05514	0.00035	0.00000	0.00101	0.00101
2.05615					
R28	2.64430	0.00162	0.00000	0.00356	0.00356
2.64786					
R29	2.05324	0.00025	0.00000	0.00072	0.00072
2.05396					
R30	2.63443	0.00152	0.00000	0.00334	0.00334
2.63777					
R31	2.05342	0.00026	0.00000	0.00074	0.00074
2.05416					
R32	2.64622	0.00165	0.00000	0.00368	0.00368
2.64990					
R33	2.05140	0.00024	0.00000	0.00067	0.00067
2.05207					
R34	2.62414	0.00000	0.00000	0.00032	0.00030
2.62444					
R35	2.26256	0.00285	0.00000	0.00268	0.00268
2.26524					
R36	2.62676	0.00065	0.00000	0.00184	0.00185
2.62861					
R37	2.26463	0.00181	0.00000	0.00172	0.00172
2.26635					
R38	2.06977	0.00026	0.00000	0.00077	0.00077
2.07055					

This journal is © The Royal Society of Chemistry 2014

R39	2.06324	0.00018	0.00000	0.00053	0.00053
2.06378					
R40	2.06955	0.00030	0.00000	0.00089	0.00089
2.07044					
A1	1.97923	0.00017	0.00000	0.00017	0.00017
1.97940					
A2	2.19676	-0.00034	0.00000	-0.00087	-0.00088
2.19588					
A3	2.10710	0.00017	0.00000	0.00074	0.00075
2.10784					
A4	1.97627	-0.00011	0.00000	-0.00202	-0.00203
1.97424					
A5	1.83516	-0.00020	0.00000	-0.00311	-0.00310
1.83206					
A6	1.88210	-0.00009	0.00000	-0.00171	-0.00171
1.88039					
A7	1.92629	0.00004	0.00000	0.00244	0.00243
1.92872					
A8	1.96669	-0.00004	0.00000	-0.00017	-0.00018
1.96651					
A9	1.86968	0.00042	0.00000	0.00471	0.00469
1.87437					
A10	1.99410	0.00001	0.00000	0.00074	0.00075
1.99485					
A11	2.08582	-0.00006	0.00000	-0.00077	-0.00077
2.08505					
A12	2.20326	0.00006	0.00000	0.00004	0.00003
2.20329					
A13	1.90273	-0.00012	0.00000	-0.00144	-0.00142
1.90131					
A14	1.91615	-0.00005	0.00000	0.00063	0.00063
1.91678					
A15	1.95602	0.00042	0.00000	0.00521	0.00518
1.96120					
A16	1.96936	0.00010	0.00000	-0.00125	-0.00127
1.96809					
A17	1.89015	-0.00031	0.00000	-0.00344	-0.00344
1.88671					
A18	1.82941	-0.00003	0.00000	0.00045	0.00048
1.82989					
A19	1.98453	0.00001	0.00000	0.00043	0.00042
1.98495					
A20	2.19349	-0.00013	0.00000	-0.00070	-0.00071
2.19278					
A21	2.10509	0.00012	0.00000	0.00034	0.00033
2.10542					
A22	1.98889	-0.00001	0.00000	0.00041	0.00040
1.98929					
A23	2.08838	-0.00003	0.00000	-0.00029	-0.00029
2.08809					
A24	2.20570	0.00004	0.00000	-0.00003	-0.00003
2.20566					

This journal is © The Royal Society of Chemistry 2014

A25	1.85916	-0.00015	0.00000	-0.00212	-0.00211
1.85705					
A26	1.81927	-0.00022	0.00000	-0.00326	-0.00325
1.81602					
A27	1.98691	-0.00001	0.00000	-0.00202	-0.00202
1.98489					
A28	1.83901	0.00025	0.00000	0.00376	0.00375
1.84276					
A29	1.99847	-0.00002	0.00000	0.00033	0.00032
1.99879					
A30	1.94617	0.00015	0.00000	0.00324	0.00323
1.94940					
A31	1.93655	-0.00013	0.00000	-0.00079	-0.00080
1.93575					
A32	1.96475	0.00009	0.00000	-0.00184	-0.00186
1.96288					
A33	1.81404	-0.00021	0.00000	-0.00066	-0.00061
1.81344					
A34	1.88621	-0.00014	0.00000	-0.00179	-0.00178
1.88443					
A35	1.98207	0.00066	0.00000	0.00811	0.00807
1.99014					
A36	1.88064	-0.00026	0.00000	-0.00291	-0.00293
1.87771					
A37	2.09587	0.00005	0.00000	0.00029	0.00029
2.09616					
A38	2.08536	0.00004	0.00000	0.00026	0.00026
2.08562					
A39	2.10196	-0.00009	0.00000	-0.00055	-0.00055
2.10141					
A40	2.10483	0.00008	0.00000	0.00059	0.00059
2.10542					
A41	2.08885	0.00011	0.00000	0.00054	0.00054
2.08939					
A42	2.08950	-0.00019	0.00000	-0.00113	-0.00113
2.08837					
A43	2.08670	0.00007	0.00000	0.00027	0.00027
2.08696					
A44	2.10253	-0.00010	0.00000	-0.00036	-0.00036
2.10218					
A45	2.09395	0.00004	0.00000	0.00009	0.00009
2.09403					
A46	2.09608	-0.00013	0.00000	-0.00046	-0.00046
2.09562					
A47	2.09128	0.00008	0.00000	0.00034	0.00034
2.09162					
A48	2.09582	0.00005	0.00000	0.00012	0.00012
2.09594					
A49	2.09649	0.00007	0.00000	0.00050	0.00050
2.09699					
A50	2.08592	0.00005	0.00000	0.00014	0.00014
2.08606					

This journal is © The Royal Society of Chemistry 2014

A51	2.10076	-0.00012	0.00000	-0.00065	-0.00065	2.10011
A52	2.09222	0.00011	0.00000	0.00044	0.00044	2.09266
A53	2.09454	-0.00017	0.00000	-0.00055	-0.00055	2.09400
A54	2.09642	0.00006	0.00000	0.00011	0.00011	2.09652
A55	2.09415	0.00004	0.00000	0.00000	0.00000	2.09415
A56	2.10232	-0.00013	0.00000	-0.00028	-0.00028	2.10204
A57	2.08671	0.00009	0.00000	0.00028	0.00028	2.08699
A58	2.09064	0.00014	0.00000	0.00071	0.00071	2.09135
A59	2.10606	0.00011	0.00000	0.00074	0.00074	2.10680
A60	2.08647	-0.00025	0.00000	-0.00146	-0.00146	2.08501
A61	1.91502	0.00024	0.00000	0.00010	-0.00006	1.91496
A62	2.24421	0.00046	0.00000	0.00234	0.00205	2.24626
A63	2.12394	-0.00069	0.00000	-0.00226	-0.00254	2.12140
A64	1.91986	0.00007	0.00000	-0.00011	-0.00030	1.91957
A65	2.25292	0.00051	0.00000	0.00196	0.00158	2.25450
A66	2.11032	-0.00058	0.00000	-0.00240	-0.00278	2.10754
A67	1.94643	-0.00007	0.00000	0.00025	0.00041	1.94683
A68	1.93112	0.00012	0.00000	0.00104	0.00104	1.93216
A69	1.93870	0.00053	0.00000	0.00324	0.00323	1.94194
A70	1.93280	0.00004	0.00000	0.00011	0.00011	1.93291
A71	1.87597	-0.00031	0.00000	-0.00158	-0.00158	1.87439
A72	1.88511	-0.00007	0.00000	-0.00025	-0.00025	1.88486
A73	1.89828	-0.00036	0.00000	-0.00275	-0.00275	1.89552
D1	3.12904	-0.00010	0.00000	-0.00128	-0.00128	3.12776
D2	-1.04979	-0.00024	0.00000	-0.00148	-0.00148	-1.05127
D3	0.94078	0.00010	0.00000	0.00165	0.00165	0.94243

This journal is © The Royal Society of Chemistry 2014

D4	-0.02741	-0.00001	0.00000	0.00187	0.00187	-0.02554
D5	2.07694	-0.00015	0.00000	0.00167	0.00167	2.07861
D6	-2.21567	0.00019	0.00000	0.00480	0.00480	-2.21087
D7	-0.00696	-0.00001	0.00000	-0.00095	-0.00095	-0.00791
D8	3.13051	0.00008	0.00000	0.00289	0.00289	3.13340
D9	-3.13454	-0.00009	0.00000	-0.00391	-0.00391	-3.13845
D10	0.00293	0.00000	0.00000	-0.00007	-0.00007	0.00286
D11	0.01413	-0.00006	0.00000	-0.00196	-0.00196	0.01218
D12	-3.13328	-0.00009	0.00000	-0.00303	-0.00303	-3.13632
D13	3.13986	0.00003	0.00000	0.00140	0.00140	3.14126
D14	-0.00756	0.00001	0.00000	0.00032	0.00032	-0.00723
D15	-1.13582	0.00013	0.00000	0.00487	0.00488	-1.13094
D16	1.02969	0.00015	0.00000	0.00277	0.00276	1.03245
D17	3.05516	0.00033	0.00000	0.00684	0.00687	3.06203
D18	1.00115	-0.00009	0.00000	0.00189	0.00189	1.00304
D19	-3.11652	-0.00008	0.00000	-0.00021	-0.00023	-3.11675
D20	-1.09105	0.00011	0.00000	0.00386	0.00388	-1.08717
D21	-3.13505	0.00015	0.00000	0.00619	0.00620	-3.12885
D22	-0.96954	0.00016	0.00000	0.00409	0.00408	-0.96546
D23	1.05593	0.00035	0.00000	0.00816	0.00819	1.06412
D24	-0.93336	-0.00003	0.00000	-0.00146	-0.00146	-0.93482
D25	2.22213	-0.00011	0.00000	-0.00669	-0.00669	2.21543
D26	-3.12731	0.00021	0.00000	0.00254	0.00254	-3.12476
D27	0.02818	0.00013	0.00000	-0.00269	-0.00269	0.02550
D28	1.03411	-0.00011	0.00000	-0.00360	-0.00359	1.03052
D29	-2.09358	-0.00018	0.00000	-0.00883	-0.00882	-2.10240

This journal is © The Royal Society of Chemistry 2014

D30	-0.91677	0.00003	0.00000	0.00040	0.00040	-0.91637
D31	1.02276	0.00015	0.00000	0.00241	0.00240	1.02517
D32	-3.13615	0.00018	0.00000	0.00305	0.00304	-3.13311
D33	2.22927	-0.00008	0.00000	-0.00374	-0.00374	2.22553
D34	-2.11438	0.00005	0.00000	-0.00173	-0.00174	-2.11612
D35	0.00989	0.00008	0.00000	-0.00110	-0.00110	0.00879
D36	0.00356	-0.00001	0.00000	-0.00007	-0.00006	0.00349
D37	3.13899	-0.00005	0.00000	-0.00186	-0.00186	3.13713
D38	3.14049	0.00010	0.00000	0.00428	0.00427	3.13842
D39	-0.00726	0.00006	0.00000	0.00248	0.00248	-0.00479
D40	-0.02830	-0.00009	0.00000	-0.00138	-0.00138	-0.02969
D41	-2.14471	0.00013	0.00000	0.00279	0.00278	-2.14193
D42	2.10833	0.00051	0.00000	0.00751	0.00749	2.11582
D43	2.09788	-0.00020	0.00000	-0.00363	-0.00362	2.09426
D44	-0.01852	0.00001	0.00000	0.00054	0.00054	-0.01798
D45	-2.04867	0.00039	0.00000	0.00526	0.00526	-2.04342
D46	-2.13226	-0.00054	0.00000	-0.00813	-0.00812	-2.14038
D47	2.03452	-0.00032	0.00000	-0.00397	-0.00396	2.03056
D48	0.00437	0.00006	0.00000	0.00076	0.00075	0.00512
D49	-2.07977	-0.00024	0.00000	-0.01290	-0.01290	-2.09267
D50	1.05691	0.00013	0.00000	0.02813	0.02814	1.08505
D51	2.10388	-0.00014	0.00000	-0.01206	-0.01205	2.09183
D52	-1.04263	0.00023	0.00000	0.02897	0.02899	-1.01364
D53	-0.00245	-0.00009	0.00000	-0.00912	-0.00910	-0.01155
D54	3.13422	0.00028	0.00000	0.03191	0.03194	-3.11702
D55	-0.01037	0.00004	0.00000	0.00029	0.00029	-0.01008

This journal is © The Royal Society of Chemistry 2014

D56	-3.13101	-0.00004	0.00000	-0.00371	-0.00372	-3.13473
D57	3.11810	0.00010	0.00000	0.00522	0.00522	3.12332
D58	-0.00253	0.00002	0.00000	0.00121	0.00121	-0.00132
D59	-0.00359	0.00009	0.00000	0.00540	0.00540	0.00181
D60	3.13704	0.00005	0.00000	0.00367	0.00367	3.14071
D61	-3.13040	0.00001	0.00000	-0.00016	-0.00016	-3.13056
D62	0.01023	-0.00003	0.00000	-0.00190	-0.00190	0.00834
D63	0.92422	-0.00007	0.00000	-0.00027	-0.00027	0.92395
D64	-1.00153	0.00013	0.00000	0.00266	0.00265	-0.99888
D65	3.13671	-0.00023	0.00000	-0.00434	-0.00435	3.13236
D66	-2.23999	0.00002	0.00000	0.00405	0.00406	-2.23593
D67	2.11744	0.00022	0.00000	0.00698	0.00698	2.12442
D68	-0.02750	-0.00014	0.00000	-0.00002	-0.00003	-0.02753
D69	3.13254	-0.00003	0.00000	-0.00142	-0.00142	3.13112
D70	-0.00727	0.00001	0.00000	0.00051	0.00051	-0.00676
D71	0.01473	-0.00013	0.00000	-0.00597	-0.00597	0.00876
D72	-3.12508	-0.00009	0.00000	-0.00405	-0.00405	-3.12912
D73	-0.96384	0.00001	0.00000	-0.00011	-0.00010	-0.96394
D74	1.19812	-0.00006	0.00000	-0.00414	-0.00415	1.19397
D75	-2.99963	-0.00006	0.00000	-0.00399	-0.00403	-3.00366
D76	0.99027	-0.00015	0.00000	-0.00230	-0.00230	0.98798
D77	-3.13095	-0.00022	0.00000	-0.00634	-0.00635	-3.13730
D78	-1.04552	-0.00022	0.00000	-0.00618	-0.00622	-1.05174
D79	-3.11485	0.00008	0.00000	0.00260	0.00262	-3.11223
D80	-0.95289	0.00002	0.00000	-0.00144	-0.00143	-0.95433
D81	1.13255	0.00001	0.00000	-0.00128	-0.00131	1.13124

This journal is © The Royal Society of Chemistry 2014

D82	-1.01151	-0.00009	0.00000	-0.01879	-0.01879	-1.03030
D83	-3.09364	-0.00013	0.00000	-0.01959	-0.01959	-3.11323
D84	1.07823	-0.00006	0.00000	-0.01836	-0.01836	1.05987
D85	3.12674	0.00015	0.00000	-0.01449	-0.01449	3.11225
D86	1.04461	0.00010	0.00000	-0.01528	-0.01529	1.02932
D87	-1.06671	0.00017	0.00000	-0.01405	-0.01405	-1.08077
D88	1.04081	-0.00027	0.00000	-0.02206	-0.02206	1.01875
D89	-1.04132	-0.00032	0.00000	-0.02286	-0.02286	-1.06418
D90	3.13054	-0.00025	0.00000	-0.02163	-0.02162	3.10892
D91	-0.00510	-0.00001	0.00000	0.00782	0.00780	0.00271
D92	3.12300	-0.00032	0.00000	-0.03959	-0.03962	3.08338
D93	2.10119	0.00006	0.00000	0.01087	0.01087	2.11206
D94	-1.05390	-0.00026	0.00000	-0.03655	-0.03655	-1.09046
D95	-2.09339	0.00011	0.00000	0.01163	0.01161	-2.08177
D96	1.03471	-0.00020	0.00000	-0.03578	-0.03581	0.99890
D97	-0.00813	0.00001	0.00000	0.00087	0.00087	-0.00726
D98	3.13649	0.00005	0.00000	0.00230	0.00230	3.13879
D99	3.13250	-0.00003	0.00000	-0.00087	-0.00087	3.13163
D100	-0.00606	0.00001	0.00000	0.00056	0.00056	-0.00550
D101	-3.13647	-0.00004	0.00000	-0.00207	-0.00207	-3.13854
D102	0.00938	-0.00003	0.00000	-0.00153	-0.00153	0.00785
D103	0.00689	0.00000	0.00000	-0.00016	-0.00016	0.00673
D104	-3.13044	0.00001	0.00000	0.00037	0.00037	-3.13007
D105	-0.00165	0.00002	0.00000	0.00084	0.00084	-0.00081
D106	3.13691	-0.00002	0.00000	-0.00059	-0.00059	3.13632
D107	-3.13896	0.00003	0.00000	0.00138	0.00138	-3.13758

```
   D108      -0.00041   0.00000   0.00000  -0.00005  -0.00005  -
0.00046
   D109      -3.13388   0.00001   0.00000   0.00065   0.00065  -
3.13322
   D110       0.00570  -0.00002   0.00000  -0.00045  -0.00045
0.00525
   D111       0.00188  -0.00001   0.00000  -0.00042  -0.00042
0.00146
   D112       3.14146  -0.00004   0.00000  -0.00153  -0.00153
3.13993
   D113      -3.13906   0.00003   0.00000   0.00110   0.00110  -
3.13796
   D114       0.00074   0.00001   0.00000   0.00032   0.00032
0.00106
   D115       0.00052   0.00000   0.00000  -0.00001  -0.00001
0.00051
   D116       3.14032  -0.00002   0.00000  -0.00079  -0.00079
3.13953
   D117      -0.00539   0.00000   0.00000  -0.00006  -0.00006  -
0.00545
   D118      -3.14090   0.00004   0.00000   0.00171   0.00171  -
3.13919
   D119       3.13441  -0.00002   0.00000  -0.00084  -0.00084
3.13358
   D120      -0.00109   0.00002   0.00000   0.00093   0.00093  -
0.00016
   D121      -0.00079   0.00009   0.00000   0.01482   0.01479
0.01400
   D122      -3.13786  -0.00025   0.00000  -0.02289  -0.02281
3.12251
   D123       0.00382  -0.00005   0.00000  -0.01434  -0.01431  -
0.01049
   D124      -3.12556   0.00023   0.00000   0.02852   0.02843  -
3.09714
         Item               Value     Threshold  Converged?
 Maximum Force            0.002848     0.000450     NO
 RMS     Force            0.000449     0.000300     NO
 Maximum Displacement     0.113571     0.001800     NO
 RMS     Displacement     0.013786     0.001200     NO
 Predicted change in Energy=-1.182467D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.706804   -0.046888   -0.893963
      2          6           0        0.299509   -0.055006   -1.456464
      3          1           0        0.273192    0.003025   -2.547531
```

This journal is © The Royal Society of Chemistry 2014

4	6	0	1.747510	-0.103587	0.512032
5	6	0	-0.326530	-1.406263	-0.962633
6	1	0	0.220059	-2.238309	-1.417778
7	6	0	-0.470547	1.071386	-0.791978
8	6	0	-0.433261	1.030315	0.615108
9	6	0	0.365060	-0.150615	1.183623
10	6	0	-0.313905	-1.456081	0.578881
11	1	0	0.225742	-2.327425	0.965049
12	6	0	-1.175875	2.073880	-1.454519
13	1	0	-1.207421	2.091424	-2.541566
14	6	0	-1.108014	2.004056	1.351857
15	1	0	-1.098060	1.982236	2.437481
16	6	0	-1.809172	3.017692	0.685181
17	1	0	-2.331705	3.776829	1.261420
18	6	0	-1.844384	3.053690	-0.710285
19	1	0	-2.394069	3.839710	-1.221354
20	6	0	2.882134	-0.003559	-1.639548
21	1	0	2.838876	0.039804	-2.725890
22	6	0	4.118545	-0.007828	-0.980312
23	1	0	5.039609	0.033718	-1.555891
24	6	0	4.165477	-0.061619	0.413708
25	1	0	5.124517	-0.061523	0.925411
26	6	0	2.981251	-0.112897	1.162931
27	1	0	3.036198	-0.152103	2.246738
28	6	0	-1.791375	-1.538603	-1.344448
29	6	0	-1.784138	-1.621606	0.952407
30	8	0	-2.564553	-1.668289	-0.198094
31	8	0	-2.279267	-1.763518	2.035472
32	8	0	-2.280598	-1.573898	-2.438219
33	6	0	0.424299	-0.200090	2.710467
34	1	0	0.981967	-1.080710	3.048172
35	1	0	-0.576244	-0.261268	3.143894
36	1	0	0.923867	0.690061	3.108548

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515570	0.000000			
3	H	2.189068	1.092926	0.000000		
4	C	1.407726	2.444186	3.397926	0.000000	
5	C	2.446847	1.568977	2.204011	2.858889	0.000000
6	H	2.699466	2.185090	2.510526	3.257961	1.094630
7	C	2.449856	1.517659	2.185523	2.828565	2.487692
8	C	2.831526	2.450773	3.399513	2.460106	2.904750
9	C	2.475358	2.642631	3.735446	1.537665	2.580962
10	C	2.870254	2.545961	3.499732	2.466403	1.542370
11	H	3.293983	3.321605	4.215622	2.732483	2.206695
12	C	3.622391	2.590158	2.753709	4.141843	3.615900
13	H	3.972364	2.838212	2.560012	4.782693	3.937361
14	C	4.144065	3.755998	4.595333	3.647120	4.194980
15	H	4.804490	4.611547	5.536060	4.019364	4.861889
16	C	4.924168	4.298215	4.886193	4.735225	4.948222

This journal is © The Royal Society of Chemistry 2014

17	H	5.964566	5.384528	5.961140	5.679719	5.985949
18	C	4.717866	3.849293	4.143207	4.936007	4.717918
19	H	5.659504	4.741250	4.857281	5.975525	5.644634
20	C	1.392543	2.589617	2.762436	2.434476	3.566696
21	H	2.155240	2.840566	2.572139	3.419909	3.901280
22	C	2.413603	3.848894	4.152473	2.803224	4.659896
23	H	3.398858	4.741973	4.868575	3.890124	5.587571
24	C	2.784833	4.294566	4.891114	2.420328	4.886768
25	H	3.871835	5.380899	5.966644	3.402474	5.923424
26	C	2.420617	3.749177	4.595057	1.394946	4.139111
27	H	3.412091	4.605714	5.535638	2.161545	4.814657
28	C	3.829543	2.566204	2.843670	4.246116	1.519561
29	C	4.251528	3.549434	4.372826	3.869219	2.416272
30	O	4.621435	3.519804	4.045484	4.641816	2.379479
31	O	5.236141	4.665053	5.535308	4.614236	3.595754
32	O	4.540469	3.150845	3.003412	5.204945	2.454351
33	C	3.828865	4.171323	5.264089	2.567746	3.938307
34	H	4.139397	4.670071	5.743582	2.823621	4.231395
35	H	4.643550	4.687514	5.760531	3.514456	4.270473
36	H	4.144416	4.667364	5.734686	2.837281	4.746850

		6	7	8	9	10
6	H	0.000000				
7	C	3.438407	0.000000			
8	C	3.904274	1.408179	0.000000		
9	C	3.338679	2.468710	1.534641	0.000000	
10	C	2.209897	2.879563	2.489523	1.590896	0.000000
11	H	2.384499	3.888944	3.439646	2.192188	1.095256
12	C	4.532654	1.393356	2.433898	3.779239	4.163932
13	H	4.695443	2.155114	3.419044	4.623469	4.808362
14	C	5.237586	2.423276	1.395084	2.615503	3.633269
15	H	5.866298	3.413624	2.160823	2.874358	3.986391
16	C	6.013797	2.786041	2.418203	3.874777	4.718237
17	H	7.061974	3.872954	3.400757	4.764810	5.649842
18	C	5.724310	2.413220	2.800354	4.328522	4.933797
19	H	6.619257	3.398223	3.887166	5.414739	5.967690
20	C	3.482805	3.621374	4.140557	3.785179	4.152820
21	H	3.709334	3.969441	4.780195	4.630369	4.806164
22	C	4.512717	4.718044	4.933766	4.334934	4.916822
23	H	5.330032	5.658810	5.971495	5.421284	5.952887
24	C	4.864015	4.922408	4.730885	3.878640	4.694323
25	H	5.855138	5.961347	5.672504	4.767289	5.625061
26	C	4.336083	4.139941	3.642244	2.616545	3.606011
27	H	5.070658	4.798748	4.012167	2.874925	3.962991
28	C	2.130923	2.976886	3.504807	3.601093	2.426710
29	C	3.164633	3.467075	2.995217	2.614638	1.525944
30	O	3.092994	3.499054	3.533577	3.577025	2.390426
31	O	4.289171	4.393475	3.637400	3.212409	2.465527
32	O	2.781372	3.603321	4.417848	4.705633	3.603423
33	C	4.608520	3.832039	2.576788	1.528794	2.581883
34	H	4.676029	4.635522	3.518394	2.173061	2.813820
35	H	5.035041	4.156709	2.843131	2.177375	2.841776
36	H	5.436756	4.159796	2.859163	2.173554	3.540793

This journal is © The Royal Society of Chemistry 2014

		11	12	13	14	15
11	H	0.000000				
12	C	5.214434	0.000000			
13	H	5.820355	1.087646	0.000000		
14	C	4.548654	2.808064	3.895671	0.000000	
15	H	4.742751	3.893857	4.981445	1.085889	0.000000
16	C	5.726210	2.422842	3.410567	1.401263	2.156017
17	H	6.624975	3.407683	4.308979	2.155997	2.474988
18	C	6.004046	1.400292	2.164548	2.428251	3.407851
19	H	7.048214	2.157897	2.491505	3.412474	4.303130
20	C	4.386422	4.562611	4.682632	5.375900	6.033862
21	H	5.104437	4.676759	4.540445	6.005352	6.777382
22	C	4.931418	5.708700	5.933826	6.066598	6.546345
23	H	5.924816	6.542536	6.650646	7.080289	7.577250
24	C	4.578140	6.048195	6.499021	5.740805	5.998151
25	H	5.397582	7.065335	7.533163	6.579736	6.721888
26	C	3.540639	5.377243	6.010600	4.608609	4.759710
27	H	3.778018	6.032898	6.780087	4.756504	4.656595
28	C	3.166193	3.666195	3.866676	4.504162	5.213442
29	C	2.130248	4.451954	5.130989	3.709734	3.957755
30	O	3.094044	4.184597	4.633476	4.243815	4.735313
31	O	2.781882	5.303125	6.079367	4.004220	3.948105
32	O	4.293225	3.936288	3.820599	5.342413	6.149547
33	C	2.758888	5.007855	5.957969	3.008665	2.674817
34	H	2.542750	5.906094	6.789773	4.094054	3.752478
35	H	3.107982	5.192098	6.185305	2.936983	2.409278
36	H	3.766588	5.210130	6.199193	2.990165	2.491633

		16	17	18	19	20
16	C	0.000000				
17	H	1.086914	0.000000			
18	C	1.396374	2.155929	0.000000		
19	H	2.157010	2.484352	1.086817	0.000000	
20	C	6.044888	7.063360	5.705284	6.540942	0.000000
21	H	6.489035	7.523224	5.922761	6.639777	1.088067
22	C	6.860428	7.807350	6.708378	7.568077	1.401186
23	H	7.799507	8.734094	7.564697	8.358054	2.159418
24	C	6.726982	7.593792	6.861992	7.805219	2.422024
25	H	7.590476	8.392920	7.806769	8.738270	3.407441
26	C	5.742560	6.585376	6.068194	7.085336	2.806362
27	H	5.996972	6.724712	6.545318	7.579580	3.892174
28	C	4.987938	5.944436	4.636176	5.413376	4.927994
29	C	4.647055	5.434926	4.962517	5.909588	5.577670
30	O	4.827959	5.642137	4.803964	5.604835	5.874990
31	O	4.990415	5.594404	5.561817	6.481995	6.575963
32	O	5.573200	6.505399	4.958892	5.549846	5.455057
33	C	4.409569	5.050860	5.237896	6.302571	5.000221
34	H	5.492821	6.145615	6.261591	7.337370	5.171616
35	H	4.279832	4.788693	5.239450	6.259225	5.908309
36	H	4.331291	4.851677	5.275741	6.298971	5.182696

		21	22	23	24	25
21	H	0.000000				
22	C	2.164916	0.000000			

23	H	2.492420	1.086911	0.000000		
24	C	3.409873	1.395847	2.156969	0.000000	
25	H	4.308877	2.155607	2.484580	1.087014	0.000000
26	C	3.894421	2.428573	3.413257	1.402267	2.156999
27	H	4.980240	3.406779	4.302112	2.154868	2.472890
28	C	5.083205	6.115801	7.012791	6.384095	7.427220
29	C	6.136971	6.417270	7.456217	6.174275	7.082662
30	O	6.205189	6.930569	7.909722	6.946149	7.935097
31	O	7.219275	7.287620	8.348286	6.860124	7.677568
32	O	5.375482	6.747378	7.546414	7.209186	8.272667
33	C	5.953294	5.225540	6.289480	4.392116	5.029680
34	H	6.167938	5.217076	6.237291	4.256017	4.765038
35	H	6.797651	6.254147	7.328902	5.475189	6.120478
36	H	6.175011	5.235628	6.255167	4.281965	4.793374

		26	27	28	29	30
26	C	0.000000				
27	H	1.085907	0.000000			
28	C	5.576518	6.174501	0.000000		
29	C	5.002945	5.202920	2.298367	0.000000	
30	O	5.918410	6.296383	1.388794	1.391000	0.000000
31	O	5.582019	5.558369	3.422351	1.199300	2.253725
32	O	6.541396	7.227631	1.198716	3.427112	2.260021
33	C	2.990063	2.653180	4.810735	3.160487	4.421377
34	H	2.913406	2.392588	5.214998	3.512283	4.843686
35	H	4.074555	3.723781	4.822173	2.848182	4.135453
36	H	2.943297	2.431852	5.671742	4.162455	5.353949

		31	32	33	34	35
31	O	0.000000				
32	O	4.477708	0.000000			
33	C	3.195183	5.976018	0.000000		
34	H	3.482446	6.402191	1.095686	0.000000	
35	H	2.526983	5.982291	1.092103	1.763141	0.000000
36	H	4.175117	6.794169	1.095630	1.772752	1.776684

		36
36	H	0.000000

Stoichiometry C19H14O3
Framework group C1[X(C19H14O3)]
Deg. of freedom 102
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.706912	-0.068555	-0.893261
2	6	0	0.299455	-0.066650	-1.455412
3	1	0	0.273466	-0.018529	-2.546968
4	6	0	1.747394	-0.112559	0.513195
5	6	0	-0.341074	-1.406360	-0.948867
6	1	0	0.196325	-2.248505	-1.396316

7	6	0	-0.458145	1.074192	-0.801341
8	6	0	-0.420914	1.045863	0.606061
9	6	0	0.364703	-0.138303	1.185442
10	6	0	-0.328560	-1.441913	0.593043
11	1	0	0.201706	-2.315419	0.987239
12	6	0	-1.152736	2.078052	-1.473092
13	1	0	-1.184393	2.085784	-2.560250
14	6	0	-1.084854	2.033709	1.333801
15	1	0	-1.074834	2.021922	2.419580
16	6	0	-1.775156	3.048625	0.657809
17	1	0	-2.289258	3.818739	1.227024
18	6	0	-1.810364	3.071969	-0.737926
19	1	0	-2.351629	3.859102	-1.256217
20	6	0	2.882435	-0.044952	-1.639427
21	1	0	2.839348	-0.011271	-2.726119
22	6	0	4.118911	-0.056485	-0.980400
23	1	0	5.040211	-0.030318	-1.556505
24	6	0	4.165646	-0.097761	0.414054
25	1	0	5.124774	-0.103296	0.925563
26	6	0	2.981143	-0.129181	1.163934
27	1	0	3.035964	-0.158857	2.248050
28	6	0	-1.807375	-1.526351	-1.329169
29	6	0	-1.800398	-1.587973	0.968361
30	8	0	-2.581595	-1.636924	-0.181516
31	8	0	-2.296736	-1.714380	2.052792
32	8	0	-2.297258	-1.566547	-2.422475
33	6	0	0.423827	-0.174156	2.712671
34	1	0	0.971998	-1.057585	3.058489
35	1	0	-0.577200	-0.220419	3.146829
36	1	0	0.933137	0.714199	3.102330

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.4226602      0.2800949
0.2676465
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   446 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   446 basis functions,   760 primitive gaussians,   446 cartesian
basis functions
    76 alpha electrons       76 beta electrons
       nuclear repulsion energy      1805.0419015660 Hartrees.
 NAtoms=   36 NActive=   36 NUniq=   36 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   446 RedAO= T  NBF=   446
 NBsUse=   441 1.00D-06 NBFU=   441
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
```

Supplementary Material (ESI) for Green Chemistry
This journal is © The Royal Society of Chemistry 2014

```
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
```

This journal is © The Royal Society of Chemistry 2014

```
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -958.192507064     A.U. after   14 cycles
             Convg  =    0.7607D-08             -V/T =  2.0094
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6           0.000339499   -0.000019719    0.000269841
      2          6           0.000084581   -0.000107229    0.000121193
      3          1          -0.000018803   -0.000015724   -0.000000788
      4          6           0.000319737    0.000085621   -0.000155997
      5          6          -0.000393052    0.001846401   -0.000245817
      6          1          -0.000229626    0.000009777   -0.000158000
      7          6          -0.000127192   -0.000214569    0.000108186
      8          6          -0.000156502   -0.000197883   -0.000065892
      9          6           0.000177987   -0.000065327   -0.000161554
     10          6          -0.000199644    0.001883567    0.000267504
     11          1          -0.000310833    0.000015685    0.000195551
     12          6           0.000017291   -0.000027995    0.000072996
     13          1          -0.000010793    0.000010420    0.000030177
     14          6           0.000001361   -0.000049867   -0.000085721
     15          1          -0.000014504    0.000051480   -0.000018229
     16          6           0.000080272   -0.000059095    0.000012588
     17          1           0.000041698   -0.000029014   -0.000016362
     18          6           0.000058861   -0.000051229   -0.000022118
     19          1           0.000047842   -0.000017928    0.000026117
     20          6          -0.000056217    0.000024436    0.000097503
     21          1           0.000009715   -0.000006406    0.000049247
     22          6          -0.000071451    0.000004733    0.000040881
     23          1          -0.000042348   -0.000008825    0.000025317
     24          6          -0.000083023   -0.000009045   -0.000026916
     25          1          -0.000056326   -0.000018718   -0.000006778
     26          6          -0.000069604    0.000014704   -0.000120368
     27          1           0.000072368   -0.000058809   -0.000035459
     28          6           0.000816224   -0.003850026    0.000582214
     29          6           0.000992638   -0.004516400   -0.000071996
     30          8          -0.000466556    0.002382230   -0.000296332
     31          8          -0.000005123    0.001809595    0.000337603
     32          8          -0.000336441    0.001398217   -0.000403008
     33          6           0.000011561   -0.000199333   -0.000471272
     34          1          -0.000104690   -0.000014387    0.000006942
     35          1          -0.000191211   -0.000038568    0.000146035
     36          1          -0.000127694    0.000039232   -0.000027290
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.004516400 RMS     0.000728602
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.001005592 RMS     0.000218121
 Search for a local minimum.
 Step number   2 out of a maximum of  216
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2
 DE=  1.83D-05 DEPred=-1.18D-04 R=-1.55D-01
 Trust test=-1.55D-01 RLast= 1.18D-01 DXMaxT set to 1.50D-01
     Eigenvalues ---    0.00375   0.00430   0.00782   0.01094
0.01126
     Eigenvalues ---    0.01161   0.01421   0.01482   0.01560
0.01786
     Eigenvalues ---    0.02051   0.02113   0.02119   0.02127
0.02130
     Eigenvalues ---    0.02131   0.02135   0.02141   0.02152
0.02157
     Eigenvalues ---    0.02158   0.02166   0.02250   0.03012
0.03419
     Eigenvalues ---    0.04160   0.04593   0.05097   0.05220
0.05240
     Eigenvalues ---    0.05379   0.05518   0.05610   0.05824
0.06390
     Eigenvalues ---    0.08046   0.08528   0.09308   0.09902
0.12677
     Eigenvalues ---    0.15730   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16004   0.16444   0.20278   0.20960
0.22000
     Eigenvalues ---    0.22000   0.22382   0.22612   0.22633
0.24269
     Eigenvalues ---    0.24572   0.24590   0.24851   0.25000
0.26182
     Eigenvalues ---    0.27467   0.27635   0.28781   0.28965
0.29644
     Eigenvalues ---    0.29775   0.30133   0.34137   0.34215
0.34255
     Eigenvalues ---    0.34317   0.34492   0.34574   0.35033
0.35125
     Eigenvalues ---    0.35190   0.35211   0.35218   0.35227
0.35318
     Eigenvalues ---    0.35336   0.36679   0.39922   0.41192
0.42011
```

```
     Eigenvalues ---    0.42043   0.43540   0.44151   0.45324
0.46026
     Eigenvalues ---    0.46102   0.46211   0.46356   0.46429
0.46855
     Eigenvalues ---    1.03131
1.058131000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     2    1
 RFO step:  Lambda=-5.35712720D-05.
 DIIS coeffs:      0.46213      0.53787
 Iteration  1 RMS(Cart)=  0.00554194 RMS(Int)=  0.00007881
 Iteration  2 RMS(Cart)=  0.00006766 RMS(Int)=  0.00004412
 Iteration  3 RMS(Cart)=  0.00000001 RMS(Int)=  0.00004412
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86401   0.00017   0.00024   0.00006   0.00029
2.86431
    R2        2.66022  -0.00027  -0.00100   0.00207   0.00107
2.66129
    R3        2.63152  -0.00018  -0.00175   0.00386   0.00211
2.63363
    R4        2.06533   0.00000  -0.00025   0.00058   0.00033
2.06566
    R5        2.96494  -0.00022  -0.00159   0.00328   0.00168
2.96662
    R6        2.86796  -0.00028  -0.00037   0.00029  -0.00008
2.86788
    R7        2.90577   0.00018  -0.00097   0.00221   0.00124
2.90700
    R8        2.63607  -0.00014  -0.00178   0.00394   0.00216
2.63823
    R9        2.06855  -0.00005  -0.00044   0.00094   0.00050
2.06905
   R10        2.91466   0.00021  -0.00140   0.00348   0.00208
2.91674
   R11        2.87155  -0.00021   0.00020  -0.00058  -0.00041
2.87114
   R12        2.66107  -0.00028  -0.00089   0.00176   0.00086
2.66194
   R13        2.63306  -0.00014  -0.00163   0.00361   0.00198
2.63504
   R14        2.90005  -0.00028  -0.00100   0.00204   0.00103
2.90108
   R15        2.63633  -0.00012  -0.00159   0.00355   0.00196
2.63829
   R16        3.00636  -0.00065  -0.00254   0.00456   0.00202
3.00838
   R17        2.88900  -0.00035  -0.00107   0.00191   0.00084
2.88985
   R18        2.06973  -0.00009  -0.00044   0.00088   0.00045
2.07018
```

R19	2.88362	-0.00053	-0.00052	0.00018	-0.00031
2.88331					
R20	2.05535	-0.00003	-0.00055	0.00123	0.00068
2.05603					
R21	2.64617	-0.00015	-0.00171	0.00379	0.00208
2.64825					
R22	2.05203	-0.00002	-0.00042	0.00094	0.00052
2.05255					
R23	2.64800	-0.00015	-0.00173	0.00384	0.00211
2.65011					
R24	2.05397	-0.00005	-0.00041	0.00088	0.00047
2.05444					
R25	2.63877	-0.00009	-0.00182	0.00413	0.00231
2.64107					
R26	2.05379	-0.00005	-0.00040	0.00086	0.00046
2.05425					
R27	2.05615	-0.00005	-0.00054	0.00118	0.00064
2.05679					
R28	2.64786	-0.00014	-0.00191	0.00429	0.00238
2.65023					
R29	2.05396	-0.00005	-0.00039	0.00083	0.00044
2.05440					
R30	2.63777	-0.00013	-0.00180	0.00402	0.00222
2.63999					
R31	2.05416	-0.00005	-0.00040	0.00085	0.00045
2.05461					
R32	2.64990	-0.00016	-0.00198	0.00439	0.00241
2.65231					
R33	2.05207	-0.00003	-0.00036	0.00079	0.00043
2.05250					
R34	2.62444	-0.00002	-0.00016	0.00043	0.00025
2.62469					
R35	2.26524	0.00046	-0.00144	0.00352	0.00208
2.26733					
R36	2.62861	0.00033	-0.00100	0.00255	0.00157
2.63018					
R37	2.26635	0.00009	-0.00092	0.00217	0.00125
2.26759					
R38	2.07055	-0.00004	-0.00042	0.00090	0.00049
2.07103					
R39	2.06378	0.00023	-0.00029	0.00097	0.00069
2.06446					
R40	2.07044	-0.00003	-0.00048	0.00105	0.00058
2.07102					
A1	1.97940	-0.00006	-0.00009	0.00042	0.00032
1.97972					
A2	2.19588	0.00001	0.00047	-0.00121	-0.00074
2.19515					
A3	2.10784	0.00005	-0.00040	0.00084	0.00044
2.10828					
A4	1.97424	0.00000	0.00109	-0.00245	-0.00136
1.97288					

This journal is © The Royal Society of Chemistry 2014

A5	1.83206	0.00010	0.00167	-0.00284	-0.00118
1.83088					
A6	1.88039	0.00003	0.00092	-0.00186	-0.00094
1.87945					
A7	1.92872	0.00000	-0.00131	0.00288	0.00157
1.93029					
A8	1.96651	-0.00001	0.00010	-0.00033	-0.00023
1.96628					
A9	1.87437	-0.00012	-0.00252	0.00472	0.00220
1.87658					
A10	1.99485	-0.00005	-0.00040	0.00039	-0.00001
1.99484					
A11	2.08505	0.00000	0.00041	-0.00080	-0.00038
2.08467					
A12	2.20329	0.00006	-0.00002	0.00041	0.00039
2.20368					
A13	1.90131	-0.00007	0.00077	-0.00214	-0.00138
1.89993					
A14	1.91678	-0.00007	-0.00034	0.00040	0.00006
1.91685					
A15	1.96120	0.00021	-0.00279	0.00732	0.00454
1.96574					
A16	1.96809	0.00013	0.00068	-0.00039	0.00030
1.96840					
A17	1.88671	-0.00010	0.00185	-0.00516	-0.00330
1.88341					
A18	1.82989	-0.00009	-0.00026	0.00019	-0.00009
1.82980					
A19	1.98495	0.00005	-0.00023	0.00036	0.00013
1.98508					
A20	2.19278	-0.00009	0.00038	-0.00086	-0.00049
2.19229					
A21	2.10542	0.00004	-0.00018	0.00056	0.00038
2.10580					
A22	1.98929	-0.00002	-0.00022	0.00057	0.00035
1.98964					
A23	2.08809	0.00002	0.00016	-0.00041	-0.00025
2.08784					
A24	2.20566	0.00000	0.00002	-0.00005	-0.00004
2.20563					
A25	1.85705	0.00004	0.00114	-0.00207	-0.00094
1.85611					
A26	1.81602	0.00013	0.00175	-0.00415	-0.00240
1.81362					
A27	1.98489	0.00010	0.00109	-0.00134	-0.00025
1.98464					
A28	1.84276	0.00003	-0.00202	0.00477	0.00277
1.84553					
A29	1.99879	-0.00001	-0.00017	0.00004	-0.00013
1.99866					
A30	1.94940	-0.00027	-0.00174	0.00263	0.00089
1.95029					

This journal is © The Royal Society of Chemistry 2014

A31	1.93575	-0.00005	0.00043	-0.00074	-0.00032
1.93542					
A32	1.96288	0.00021	0.00100	-0.00064	0.00038
1.96326					
A33	1.81344	0.00011	0.00033	-0.00059	-0.00026
1.81318					
A34	1.88443	-0.00004	0.00095	-0.00239	-0.00144
1.88300					
A35	1.99014	-0.00001	-0.00434	0.00963	0.00529
1.99544					
A36	1.87771	-0.00021	0.00157	-0.00516	-0.00359
1.87413					
A37	2.09616	0.00002	-0.00016	0.00044	0.00028
2.09644					
A38	2.08562	-0.00002	-0.00014	0.00024	0.00010
2.08572					
A39	2.10141	-0.00001	0.00030	-0.00069	-0.00039
2.10102					
A40	2.10542	0.00006	-0.00032	0.00091	0.00059
2.10601					
A41	2.08939	-0.00002	-0.00029	0.00063	0.00034
2.08973					
A42	2.08837	-0.00004	0.00061	-0.00154	-0.00093
2.08744					
A43	2.08696	-0.00001	-0.00014	0.00028	0.00014
2.08711					
A44	2.10218	0.00000	0.00019	-0.00040	-0.00021
2.10197					
A45	2.09403	0.00001	-0.00005	0.00011	0.00007
2.09410					
A46	2.09562	-0.00002	0.00025	-0.00060	-0.00036
2.09527					
A47	2.09162	0.00001	-0.00018	0.00043	0.00025
2.09187					
A48	2.09594	0.00001	-0.00006	0.00016	0.00010
2.09604					
A49	2.09699	0.00002	-0.00027	0.00064	0.00037
2.09736					
A50	2.08606	-0.00002	-0.00008	0.00019	0.00011
2.08617					
A51	2.10011	0.00000	0.00035	-0.00083	-0.00048
2.09963					
A52	2.09266	0.00001	-0.00023	0.00053	0.00030
2.09296					
A53	2.09400	-0.00002	0.00029	-0.00066	-0.00037
2.09363					
A54	2.09652	0.00001	-0.00006	0.00013	0.00007
2.09660					
A55	2.09415	0.00002	0.00000	0.00007	0.00006
2.09421					
A56	2.10204	0.00000	0.00015	-0.00035	-0.00020
2.10184					

A57	2.08699	-0.00002	-0.00015	0.00028	0.00013	2.08712
A58	2.09135	-0.00001	-0.00038	0.00079	0.00041	2.09176
A59	2.10680	0.00008	-0.00040	0.00118	0.00078	2.10758
A60	2.08501	-0.00007	0.00078	-0.00198	-0.00120	2.08381
A61	1.91496	0.00010	0.00003	0.00061	0.00042	1.91538
A62	2.24626	-0.00001	-0.00110	0.00290	0.00167	2.24794
A63	2.12140	-0.00004	0.00137	-0.00281	-0.00156	2.11984
A64	1.91957	0.00002	0.00016	0.00022	0.00005	1.91962
A65	2.25450	-0.00024	-0.00085	0.00294	0.00174	2.25625
A66	2.10754	0.00030	0.00149	-0.00137	-0.00022	2.10732
A67	1.94683	-0.00012	-0.00022	-0.00010	-0.00036	1.94647
A68	1.93216	0.00004	-0.00056	0.00148	0.00092	1.93308
A69	1.94194	0.00006	-0.00174	0.00404	0.00230	1.94424
A70	1.93291	-0.00004	-0.00006	0.00006	0.00001	1.93291
A71	1.87439	-0.00007	0.00085	-0.00228	-0.00142	1.87296
A72	1.88486	0.00006	0.00014	0.00014	0.00027	1.88514
A73	1.89552	-0.00005	0.00148	-0.00371	-0.00223	1.89329
D1	3.12776	-0.00003	0.00069	-0.00206	-0.00137	3.12639
D2	-1.05127	0.00004	0.00079	-0.00177	-0.00098	-1.05225
D3	0.94243	-0.00003	-0.00089	0.00145	0.00057	0.94300
D4	-0.02554	-0.00001	-0.00101	0.00243	0.00142	-0.02412
D5	2.07861	0.00005	-0.00090	0.00272	0.00181	2.08043
D6	-2.21087	-0.00002	-0.00258	0.00594	0.00336	-2.20752
D7	-0.00791	0.00001	0.00051	-0.00029	0.00022	-0.00769
D8	3.13340	-0.00002	-0.00155	0.00315	0.00160	3.13499
D9	-3.13845	0.00000	0.00210	-0.00451	-0.00241	-3.14086

This journal is © The Royal Society of Chemistry 2014

D10	0.00286	-0.00003	0.00004	-0.00107	-0.00103	0.00183
D11	0.01218	0.00000	0.00105	-0.00268	-0.00163	0.01054
D12	-3.13632	0.00001	0.00163	-0.00381	-0.00218	-3.13850
D13	3.14126	0.00001	-0.00075	0.00210	0.00135	-3.14058
D14	-0.00723	0.00002	-0.00017	0.00097	0.00080	-0.00644
D15	-1.13094	-0.00012	-0.00262	0.00203	-0.00060	-1.13154
D16	1.03245	-0.00006	-0.00149	0.00038	-0.00110	1.03135
D17	3.06203	-0.00008	-0.00369	0.00530	0.00159	3.06362
D18	1.00304	-0.00006	-0.00102	-0.00107	-0.00209	1.00096
D19	-3.11675	0.00001	0.00012	-0.00272	-0.00258	-3.11933
D20	-1.08717	-0.00002	-0.00209	0.00221	0.00010	-1.08707
D21	-3.12885	-0.00015	-0.00334	0.00340	0.00005	-3.12880
D22	-0.96546	-0.00009	-0.00220	0.00175	-0.00045	-0.96590
D23	1.06412	-0.00011	-0.00441	0.00667	0.00224	1.06636
D24	-0.93482	-0.00003	0.00079	-0.00213	-0.00134	-0.93617
D25	2.21543	-0.00005	0.00360	-0.00899	-0.00539	2.21005
D26	-3.12476	-0.00004	-0.00137	0.00263	0.00125	-3.12351
D27	0.02550	-0.00006	0.00144	-0.00423	-0.00279	0.02271
D28	1.03052	0.00005	0.00193	-0.00402	-0.00209	1.02843
D29	-2.10240	0.00003	0.00474	-0.01088	-0.00613	-2.10854
D30	-0.91637	-0.00001	-0.00021	0.00016	-0.00006	-0.91643
D31	1.02517	0.00009	-0.00129	0.00295	0.00166	1.02683
D32	-3.13311	-0.00010	-0.00164	0.00264	0.00100	-3.13211
D33	2.22553	0.00002	0.00201	-0.00356	-0.00155	2.22398
D34	-2.11612	0.00012	0.00093	-0.00076	0.00018	-2.11594
D35	0.00879	-0.00006	0.00059	-0.00108	-0.00048	0.00831

This journal is © The Royal Society of Chemistry 2014

D36	0.00349	0.00002	0.00003	0.00064	0.00068	0.00417
D37	3.13713	0.00004	0.00100	-0.00103	-0.00003	3.13710
D38	-3.13842	-0.00001	-0.00230	0.00453	0.00224	-3.13619
D39	-0.00479	0.00001	-0.00133	0.00286	0.00153	-0.00326
D40	-0.02969	0.00010	0.00074	0.00221	0.00295	-0.02674
D41	-2.14193	0.00004	-0.00149	0.00626	0.00476	-2.13716
D42	2.11582	0.00013	-0.00403	0.01301	0.00897	2.12479
D43	2.09426	0.00005	0.00195	-0.00051	0.00143	2.09569
D44	-0.01798	-0.00002	-0.00029	0.00353	0.00325	-0.01473
D45	-2.04342	0.00008	-0.00283	0.01028	0.00746	-2.03596
D46	-2.14038	-0.00006	0.00437	-0.00679	-0.00242	-2.14280
D47	2.03056	-0.00013	0.00213	-0.00275	-0.00061	2.02995
D48	0.00512	-0.00003	-0.00041	0.00400	0.00360	0.00872
D49	-2.09267	0.00058	0.00694	0.00796	0.01490	-2.07777
D50	1.08505	-0.00074	-0.01514	-0.01460	-0.02976	1.05528
D51	2.09183	0.00060	0.00648	0.00954	0.01602	2.10785
D52	-1.01364	-0.00072	-0.01559	-0.01302	-0.02865	-1.04229
D53	-0.01155	0.00055	0.00489	0.01247	0.01736	0.00581
D54	-3.11702	-0.00077	-0.01718	-0.01009	-0.02731	3.13885
D55	-0.01008	0.00000	-0.00016	0.00138	0.00122	-0.00886
D56	-3.13473	-0.00001	0.00200	-0.00515	-0.00315	-3.13788
D57	3.12332	0.00001	-0.00281	0.00785	0.00504	3.12836
D58	-0.00132	0.00000	-0.00065	0.00132	0.00067	-0.00065
D59	0.00181	0.00002	-0.00291	0.00708	0.00417	0.00598
D60	3.14071	0.00004	-0.00197	0.00539	0.00342	-3.13905
D61	-3.13056	0.00000	0.00009	-0.00022	-0.00013	-3.13070

This journal is © The Royal Society of Chemistry 2014

D62	0.00834	0.00002	0.00102	-0.00190	-0.00088	0.00746
D63	0.92395	0.00004	0.00014	-0.00077	-0.00062	0.92333
D64	-0.99888	-0.00014	-0.00143	0.00273	0.00130	-0.99758
D65	3.13236	0.00019	0.00234	-0.00411	-0.00177	3.13059
D66	-2.23593	0.00005	-0.00218	0.00628	0.00410	-2.23184
D67	2.12442	-0.00013	-0.00375	0.00977	0.00602	2.13044
D68	-0.02753	0.00020	0.00001	0.00293	0.00295	-0.02458
D69	3.13112	0.00001	0.00076	-0.00105	-0.00029	3.13083
D70	-0.00676	-0.00003	-0.00027	0.00044	0.00017	-0.00660
D71	0.00876	0.00000	0.00321	-0.00847	-0.00525	0.00351
D72	-3.12912	-0.00004	0.00218	-0.00697	-0.00479	-3.13392
D73	-0.96394	-0.00011	0.00005	-0.00317	-0.00312	-0.96706
D74	1.19397	0.00010	0.00223	-0.00606	-0.00382	1.19014
D75	-3.00366	-0.00021	0.00217	-0.00821	-0.00604	-3.00970
D76	0.98798	0.00000	0.00123	-0.00531	-0.00407	0.98391
D77	-3.13730	0.00021	0.00341	-0.00820	-0.00478	3.14111
D78	-1.05174	-0.00010	0.00335	-0.01035	-0.00700	-1.05874
D79	-3.11223	-0.00017	-0.00141	-0.00037	-0.00178	-3.11401
D80	-0.95433	0.00004	0.00077	-0.00326	-0.00249	-0.95681
D81	1.13124	-0.00026	0.00070	-0.00541	-0.00471	1.12653
D82	-1.03030	0.00000	0.01011	-0.02203	-0.01193	-1.04223
D83	-3.11323	0.00003	0.01054	-0.02279	-0.01225	-3.12548
D84	1.05987	0.00008	0.00987	-0.02085	-0.01098	1.04889
D85	3.11225	-0.00012	0.00779	-0.01813	-0.01033	3.10192
D86	1.02932	-0.00009	0.00822	-0.01888	-0.01066	1.01866
D87	-1.08077	-0.00005	0.00756	-0.01694	-0.00938	-1.09015

This journal is © The Royal Society of Chemistry 2014

D88	1.01875	0.00005	0.01186	-0.02642	-0.01456	1.00419
D89	-1.06418	0.00008	0.01229	-0.02718	-0.01488	-1.07906
D90	3.10892	0.00013	0.01163	-0.02524	-0.01361	3.09531
D91	0.00271	-0.00049	-0.00420	-0.01939	-0.02357	-0.02086
D92	3.08338	0.00100	0.02131	0.01503	0.03638	3.11976
D93	2.11206	-0.00049	-0.00585	-0.01535	-0.02119	2.09087
D94	-1.09046	0.00101	0.01966	0.01907	0.03876	-1.05170
D95	-2.08177	-0.00069	-0.00625	-0.01598	-0.02222	-2.10399
D96	0.99890	0.00080	0.01926	0.01845	0.03773	1.03663
D97	-0.00726	-0.00002	-0.00047	0.00073	0.00026	-0.00700
D98	3.13879	-0.00003	-0.00124	0.00228	0.00104	3.13984
D99	3.13163	0.00000	0.00047	-0.00095	-0.00049	3.13115
D100	-0.00550	0.00000	-0.00030	0.00060	0.00029	-0.00521
D101	-3.13854	0.00003	0.00111	-0.00203	-0.00092	-3.13946
D102	0.00785	0.00003	0.00082	-0.00161	-0.00078	0.00707
D103	0.00673	-0.00001	0.00009	-0.00056	-0.00047	0.00625
D104	-3.13007	-0.00001	-0.00020	-0.00014	-0.00034	-3.13041
D105	-0.00081	0.00000	-0.00045	0.00103	0.00057	-0.00023
D106	3.13632	0.00000	0.00032	-0.00053	-0.00021	3.13611
D107	-3.13758	0.00000	-0.00074	0.00145	0.00071	-3.13687
D108	-0.00046	0.00000	0.00003	-0.00010	-0.00008	-0.00053
D109	-3.13322	-0.00001	-0.00035	0.00056	0.00021	-3.13301
D110	0.00525	0.00000	0.00024	-0.00046	-0.00021	0.00504
D111	0.00146	0.00000	0.00023	-0.00056	-0.00034	0.00112
D112	3.13993	0.00001	0.00082	-0.00158	-0.00076	3.13917
D113	-3.13796	-0.00002	-0.00059	0.00083	0.00024	-3.13772

```
   D114       0.00106  -0.00001  -0.00017   0.00004  -0.00013
0.00093
   D115       0.00051  -0.00001   0.00001  -0.00019  -0.00019
0.00032
   D116       3.13953   0.00000   0.00042  -0.00098  -0.00056
3.13897
   D117      -0.00545   0.00000   0.00003  -0.00014  -0.00011  -
0.00556
   D118      -3.13919  -0.00002  -0.00092   0.00150   0.00058  -
3.13861
   D119       3.13358   0.00001   0.00045  -0.00092  -0.00047
3.13310
   D120      -0.00016  -0.00002  -0.00050   0.00072   0.00022
0.00006
   D121       0.01400  -0.00091  -0.00795  -0.02604  -0.03396  -
0.01996
   D122       3.12251   0.00030   0.01227  -0.00524   0.00692
3.12944
   D123      -0.01049   0.00089   0.00770   0.02890   0.03656
0.02607
   D124      -3.09714  -0.00043  -0.01529  -0.00232  -0.01751  -
3.11465
         Item               Value     Threshold  Converged?
 Maximum Force            0.001006     0.000450     NO
 RMS     Force            0.000218     0.000300     YES
 Maximum Displacement     0.041970     0.001800     NO
 RMS     Displacement     0.005542     0.001200     NO
 Predicted change in Energy=-1.544319D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.704084   -0.048808   -0.894024
      2          6           0        0.296801   -0.057683   -1.456960
      3          1           0        0.272188    0.001750   -2.548167
      4          6           0        1.744917   -0.105482    0.512534
      5          6           0       -0.326934   -1.411125   -0.963362
      6          1           0        0.221716   -2.241130   -1.420387
      7          6           0       -0.472620    1.069130   -0.792551
      8          6           0       -0.436427    1.027579    0.615006
      9          6           0        0.361939   -0.153578    1.184459
     10          6           0       -0.312384   -1.462502    0.579185
     11          1           0        0.233161   -2.330907    0.964356
     12          6           0       -1.173125    2.075655   -1.456300
     13          1           0       -1.203733    2.093563   -2.543729
     14          6           0       -1.108283    2.004786    1.351775
     15          1           0       -1.099877    1.983276    2.437693
```

16	6	0	-1.805600	3.022177	0.684441
17	1	0	-2.326259	3.783026	1.260587
18	6	0	-1.839056	3.058942	-0.712270
19	1	0	-2.385536	3.847197	-1.223852
20	6	0	2.879925	-0.001654	-1.640658
21	1	0	2.836478	0.042913	-2.727284
22	6	0	4.117798	-0.002980	-0.981480
23	1	0	5.038805	0.041729	-1.557353
24	6	0	4.165130	-0.057447	0.413677
25	1	0	5.124419	-0.054863	0.925415
26	6	0	2.979930	-0.112152	1.163506
27	1	0	3.036228	-0.151230	2.247476
28	6	0	-1.791044	-1.553139	-1.343647
29	6	0	-1.780402	-1.643816	0.953421
30	8	0	-2.565000	-1.666839	-0.195959
31	8	0	-2.278993	-1.758777	2.038821
32	8	0	-2.286117	-1.565505	-2.436493
33	6	0	0.421639	-0.201594	2.711779
34	1	0	0.970047	-1.087597	3.051396
35	1	0	-0.578564	-0.251191	3.148376
36	1	0	0.930245	0.684420	3.108479

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515725	0.000000			
3	H	2.188394	1.093101	0.000000		
4	C	1.408292	2.445043	3.398282	0.000000	
5	C	2.446579	1.569869	2.206075	2.859290	0.000000
6	H	2.698286	2.185043	2.510964	3.258423	1.094895
7	C	2.449107	1.517615	2.185458	2.828503	2.490395
8	C	2.831531	2.451216	3.400018	2.460201	2.906976
9	C	2.476373	2.643962	3.736934	1.538319	2.582461
10	C	2.869673	2.547648	3.502298	2.465449	1.543471
11	H	3.290162	3.321802	4.216708	2.728016	2.208122
12	C	3.620474	2.590717	2.753577	4.141091	3.621693
13	H	3.970728	2.839107	2.560087	4.782371	3.943244
14	C	4.143702	3.757264	4.596455	3.646684	4.199859
15	H	4.805403	4.613518	5.537852	4.020199	4.866886
16	C	4.923452	4.300142	4.887733	4.734762	4.955388
17	H	5.963972	5.386702	5.962934	5.679309	5.993535
18	C	4.716460	3.850949	4.144188	4.935442	4.725576
19	H	5.657971	4.743139	4.858474	5.974893	5.652933
20	C	1.393659	2.590253	2.761136	2.436238	3.567811
21	H	2.156750	2.841444	2.570868	3.421980	3.902925
22	C	2.415732	3.850856	4.152498	2.805913	4.662493
23	H	3.401259	4.744108	4.868670	3.893045	5.590596
24	C	2.786916	4.296888	4.891934	2.422707	4.889511
25	H	3.874156	5.383457	5.967673	3.405006	5.926565
26	C	2.421823	3.750866	4.595797	1.396090	4.140803
27	H	3.413813	4.608260	5.537283	2.163238	4.817434
28	C	3.831592	2.570667	2.850522	4.247840	1.519344

This journal is © The Royal Society of Chemistry 2014

29	C	4.254262	3.555352	4.379741	3.871528	2.416769
30	O	4.618485	3.517017	4.045579	4.638447	2.379756
31	O	5.233592	4.663574	5.536103	4.610292	3.597847
32	O	4.538864	3.147137	3.002280	5.203620	2.456083
33	C	3.830121	4.173091	5.265996	2.568459	3.940811
34	H	4.145387	4.673249	5.747068	2.830335	4.231443
35	H	4.646767	4.691783	5.765272	3.516740	4.279621
36	H	4.142038	4.668534	5.735566	2.833119	4.748863
		6	7	8	9	10
6	H	0.000000				
7	C	3.440073	0.000000			
8	C	3.906460	1.408635	0.000000		
9	C	3.341072	2.469833	1.535186	0.000000	
10	C	2.211292	2.883834	2.493426	1.591965	0.000000
11	H	2.386460	3.891670	3.442357	2.192211	1.095492
12	C	4.536684	1.394404	2.435467	3.781470	4.171646
13	H	4.699293	2.156528	3.420919	4.626052	4.815879
14	C	5.242288	2.424387	1.396120	2.616884	3.640390
15	H	5.871712	3.415200	2.162339	2.876395	3.993443
16	C	6.020191	2.787962	2.420305	3.877327	4.727908
17	H	7.068964	3.875124	3.403047	4.767500	5.659997
18	C	5.730530	2.415149	2.802761	4.331541	4.943890
19	H	6.626018	3.400430	3.889817	5.418006	5.978445
20	C	3.482792	3.620141	4.140716	3.787429	4.153627
21	H	3.709691	3.968179	4.780416	4.632892	4.807738
22	C	4.514577	4.717738	4.934753	4.338254	4.918577
23	H	5.332405	5.658293	5.972371	5.424828	5.955059
24	C	4.866495	4.922691	4.732033	3.881701	4.695711
25	H	5.858245	5.961679	5.673715	4.770541	5.626735
26	C	4.337833	4.140252	3.642985	2.618403	3.606135
27	H	5.073695	4.800318	4.014210	2.877817	3.964320
28	C	2.128480	2.986343	3.511612	3.603530	2.427331
29	C	3.162314	3.481205	3.009509	2.619888	1.525779
30	O	3.097552	3.495640	3.528225	3.572462	2.391000
31	O	4.295618	4.390525	3.631264	3.206419	2.466955
32	O	2.788936	3.596194	4.411018	4.702875	3.605627
33	C	4.612426	3.833376	2.577518	1.529241	2.583919
34	H	4.678406	4.637746	3.519678	2.174314	2.810162
35	H	5.047168	4.157569	2.841376	2.179689	2.852870
36	H	5.437967	4.163420	2.864081	2.174182	3.542701
		11	12	13	14	15
11	H	0.000000				
12	C	5.220632	0.000000			
13	H	5.826427	1.088006	0.000000		
14	C	4.554975	2.809717	3.897684	0.000000	
15	H	4.749725	3.895777	4.983724	1.086164	0.000000
16	C	5.735015	2.424603	3.412572	1.402380	2.156676
17	H	6.634648	3.409738	4.311284	2.157294	2.475618
18	C	6.012955	1.401392	2.165603	2.430135	3.409649
19	H	7.057960	2.159244	2.492783	3.414631	4.305117
20	C	4.383705	4.558115	4.677791	5.374593	6.034212
21	H	5.102988	4.671655	4.534552	6.004066	6.777676

This journal is © The Royal Society of Chemistry 2014

22	C	4.929090	5.704388	5.929149	6.065240	6.546762
23	H	5.923060	6.537212	6.644715	7.078369	7.577164
24	C	4.575178	6.045155	6.495981	5.739487	5.998457
25	H	5.395026	7.061922	7.529688	6.578033	6.721820
26	C	3.536563	5.375663	6.009310	4.607642	4.760168
27	H	3.775524	6.032879	6.780265	4.756854	4.658290
28	C	3.166892	3.682752	3.883757	4.515562	5.223263
29	C	2.127592	4.473255	5.150787	3.731317	3.977685
30	O	3.101132	4.187127	4.637423	4.242444	4.733503
31	O	2.791545	5.304874	6.082473	4.000875	3.943650
32	O	4.300973	3.931611	3.817306	5.337157	6.144811
33	C	2.760976	5.010192	5.960700	3.009716	2.676526
34	H	2.538613	5.909203	6.793417	4.095242	3.753862
35	H	3.123149	5.193338	6.187792	2.932203	2.402017
36	H	3.765022	5.215066	6.203789	2.997495	2.501675

		16	17	18	19	20
16	C	0.000000				
17	H	1.087163	0.000000			
18	C	1.397594	2.157273	0.000000		
19	H	2.158371	2.485975	1.087061	0.000000	
20	C	6.041835	7.060125	5.700696	6.535477	0.000000
21	H	6.485735	7.519668	5.917545	6.633424	1.088407
22	C	6.856640	7.802985	6.703131	7.561479	1.402443
23	H	7.794523	8.728245	7.557958	8.349470	2.160923
24	C	6.723615	7.589770	6.857834	7.799934	2.423872
25	H	7.586264	8.387749	7.801781	8.731830	3.409592
26	C	5.740629	6.583121	6.066054	7.082666	2.808121
27	H	5.996406	6.723732	6.544746	7.578460	3.894148
28	C	5.004685	5.961808	4.655345	5.434281	4.930849
29	C	4.673807	5.462868	4.989379	5.937839	5.580733
30	O	4.831010	5.646198	4.809010	5.611895	5.874283
31	O	4.991590	5.596379	5.565291	6.487167	6.575749
32	O	5.569375	6.502061	4.955635	5.547767	5.455911
33	C	4.411734	5.053127	5.240797	6.305723	5.002685
34	H	5.495174	6.147812	6.264985	7.340973	5.180953
35	H	4.276860	4.784672	5.239314	6.259258	5.912551
36	H	4.338884	4.860132	5.282566	6.306081	5.179406

		21	22	23	24	25
21	H	0.000000				
22	C	2.166037	0.000000			
23	H	2.493789	1.087144	0.000000		
24	C	3.411894	1.397023	2.158264	0.000000	
25	H	4.311199	2.156902	2.486121	1.087253	0.000000
26	C	3.896520	2.430562	3.415512	1.403543	2.158426
27	H	4.982552	3.408508	4.303983	2.155465	2.473393
28	C	5.086826	6.119524	7.016845	6.387589	7.430821
29	C	6.140702	6.420666	7.459667	6.177154	7.085344
30	O	6.205387	6.931469	7.911413	6.946686	7.936190
31	O	7.220103	7.288620	8.350117	6.860199	7.678118
32	O	5.377039	6.750457	7.550534	7.212232	8.276503
33	C	5.956059	5.228882	6.293085	4.394972	5.032770
34	H	6.176954	5.229611	6.250659	4.269347	4.779659

This journal is © The Royal Society of Chemistry 2014

35	H	6.802381	6.258845	7.333793	5.478936	6.124060
36	H	6.172632	5.230753	6.250064	4.275137	4.785750

		26	27	28	29	30
26	C	0.000000				
27	H	1.086134	0.000000			
28	C	5.578930	6.177708	0.000000		
29	C	5.005087	5.205988	2.298882	0.000000	
30	O	5.917048	6.296126	1.388929	1.391833	0.000000
31	O	5.579769	5.556916	3.423664	1.199959	2.254883
32	O	6.542437	7.229598	1.199817	3.428323	2.260097
33	C	2.991656	2.655973	4.813432	3.165566	4.418359
34	H	2.924937	2.406694	5.211215	3.503690	4.835018
35	H	4.076999	3.726705	4.831506	2.863851	4.139392
36	H	2.935755	2.423799	5.677457	4.172837	5.353921

		31	32	33	34	35
31	O	0.000000				
32	O	4.479492	0.000000			
33	C	3.189217	5.974688	0.000000		
34	H	3.468724	6.399056	1.095944	0.000000	
35	H	2.528910	5.986144	1.092466	1.762718	0.000000
36	H	4.172840	6.793663	1.095935	1.773383	1.775800

		36
36	H	0.000000

Stoichiometry C19H14O3
Framework group C1[X(C19H14O3)]
Deg. of freedom 102
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.704783	-0.062402	-0.893867
2	6	0	0.297478	-0.052365	-1.456729
3	1	0	0.273573	0.009772	-2.547801
4	6	0	1.744955	-0.122677	0.512561
5	6	0	-0.343186	-1.398949	-0.966067
6	1	0	0.194979	-2.234771	-1.424951
7	6	0	-0.457705	1.082559	-0.789794
8	6	0	-0.421984	1.037461	0.617666
9	6	0	0.361507	-0.154878	1.184469
10	6	0	-0.329225	-1.453896	0.576363
11	1	0	0.205385	-2.329929	0.959588
12	6	0	-1.145539	2.099259	-1.451284
13	1	0	-1.175961	2.119941	-2.538668
14	6	0	-1.081486	2.021407	1.356625
15	1	0	-1.073310	1.997406	2.442492
16	6	0	-1.765996	3.048940	0.691574
17	1	0	-2.277037	3.814999	1.269426
18	6	0	-1.799041	3.089194	-0.705050

This journal is © The Royal Society of Chemistry 2014

```
     19          1           0       -2.335597    3.885372   -1.214863
     20          6           0        2.881095   -0.028378   -1.640472
     21          1           0        2.838171    0.019121   -2.726995
     22          6           0        4.118879   -0.046699   -0.981380
     23          1           0        5.040353   -0.012295   -1.557213
     24          6           0        4.165576   -0.104823    0.413651
     25          1           0        5.124841   -0.115413    0.925330
     26          6           0        2.979811   -0.146289    1.163435
     27          1           0        3.035655   -0.188453    2.247313
     28          6           0       -1.808979   -1.521728   -1.346567
     29          6           0       -1.799390   -1.617582    0.950296
     30          8           0       -2.584259   -1.628221   -0.199081
     31          8           0       -2.299344   -1.728658    2.035473
     32          8           0       -2.304209   -1.525471   -2.439405
     33          6           0        0.420657   -0.206999    2.711676
     34          1           0        0.957907   -1.100564    3.049308
     35          1           0       -0.580073   -0.244990    3.148228
     36          1           0        0.940366    0.671684    3.110289
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.4218546      0.2801405
0.2675143
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   446 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   446 basis functions,   760 primitive gaussians,   446 cartesian
basis functions
    76 alpha electrons       76 beta electrons
       nuclear repulsion energy      1804.2123878221 Hartrees.
 NAtoms=   36 NActive=   36 NUniq=   36 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   446 RedAO= T  NBF=   446
 NBsUse=   441 1.00D-06 NBFU=   441
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -958.192546545     A.U. after   13 cycles
             Convg  =    0.6639D-08             -V/T =  2.0095
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
```

This journal is © The Royal Society of Chemistry 2014

Number	Number	X	Y	Z
1	6	0.001128984	0.000075384	0.000264390
2	6	-0.000302225	-0.000240418	0.000045773
3	1	-0.000165951	-0.000170303	0.000147594
4	6	0.001109716	0.000070687	-0.000198014
5	6	0.000019280	-0.000335122	-0.000312512
6	1	0.000199198	0.000192362	0.000127424
7	6	-0.000533771	0.000394801	0.000177650
8	6	-0.000459518	0.000365511	-0.000018118
9	6	-0.000366261	-0.000122962	-0.000012130
10	6	0.000008634	-0.000827119	-0.000026044
11	1	0.000251549	0.000248818	-0.000108411
12	6	-0.000159617	-0.000002415	0.000831339
13	1	0.000034231	-0.000023193	0.000299367
14	6	-0.000187172	0.000033135	-0.000773851
15	1	0.000049659	-0.000003386	-0.000219547
16	6	0.000512101	-0.000729484	-0.000597978
17	1	0.000159974	-0.000160076	-0.000109236
18	6	0.000488168	-0.000792520	0.000514032
19	1	0.000170693	-0.000145899	0.000106313
20	6	0.000171927	-0.000040876	0.000941101
21	1	-0.000032578	-0.000046991	0.000306444
22	6	-0.000965285	-0.000022349	0.000580571
23	1	-0.000212987	-0.000018833	0.000106324
24	6	-0.001021671	-0.000026952	-0.000538635
25	1	-0.000238704	-0.000027492	-0.000078185
26	6	0.000077460	0.000046783	-0.000885412
27	1	-0.000060094	-0.000070977	-0.000193031
28	6	-0.000982617	0.001956362	-0.000536355
29	6	-0.000688169	0.003288295	0.000952471
30	8	0.000479840	-0.001301186	-0.000111600
31	8	0.000948772	-0.000811397	-0.000961714
32	8	0.000904811	-0.000522425	0.001078019
33	6	-0.000058633	-0.000147018	-0.000203277
34	1	-0.000028267	0.000161571	-0.000142578
35	1	-0.000098787	-0.000131333	-0.000261436
36	1	-0.000152690	-0.000112983	-0.000190749

Cartesian Forces: Max 0.003288295 RMS 0.000590465

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal Forces: Max 0.001414541 RMS 0.000367669
Search for a local minimum.
Step number 3 out of a maximum of 216
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swaping is turned off.

This journal is © The Royal Society of Chemistry 2014

```
 Update second derivatives using D2CorX and points    1    2    3
 DE= -3.95D-05 DEPred=-1.54D-04 R= 2.56D-01
 Trust test= 2.56D-01 RLast= 1.19D-01 DXMaxT set to 1.50D-01
     Eigenvalues ---    0.00399   0.00430   0.00778   0.01073
0.01139
     Eigenvalues ---    0.01160   0.01426   0.01484   0.01560
0.01787
     Eigenvalues ---    0.02112   0.02118   0.02127   0.02130
0.02131
     Eigenvalues ---    0.02134   0.02140   0.02144   0.02146
0.02157
     Eigenvalues ---    0.02160   0.02166   0.02736   0.03382
0.03738
     Eigenvalues ---    0.04191   0.04580   0.05119   0.05240
0.05363
     Eigenvalues ---    0.05458   0.05512   0.05601   0.05876
0.06394
     Eigenvalues ---    0.08109   0.08527   0.09302   0.10134
0.12690
     Eigenvalues ---    0.15786   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16019   0.16473   0.20290   0.21557
0.22000
     Eigenvalues ---    0.22001   0.22396   0.22613   0.22650
0.24541
     Eigenvalues ---    0.24588   0.24644   0.24890   0.25128
0.26341
     Eigenvalues ---    0.27441   0.27770   0.28813   0.28992
0.29718
     Eigenvalues ---    0.29827   0.30425   0.34211   0.34223
0.34252
     Eigenvalues ---    0.34316   0.34506   0.34564   0.35109
0.35156
     Eigenvalues ---    0.35209   0.35218   0.35226   0.35280
0.35335
     Eigenvalues ---    0.35368   0.36673   0.39872   0.42003
0.42045
     Eigenvalues ---    0.43290   0.44054   0.44885   0.45651
0.46027
     Eigenvalues ---    0.46159   0.46356   0.46403   0.46848
0.49072
     Eigenvalues ---    1.03093
1.058401000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     3    2    1
 RFO step:  Lambda=-5.94251566D-05.
 DIIS coeffs:      0.40641      0.27941      0.31418
 Iteration  1 RMS(Cart)=  0.00541831 RMS(Int)=  0.00002347
 Iteration  2 RMS(Cart)=  0.00002348 RMS(Int)=  0.00001089
```

This journal is © The Royal Society of Chemistry 2014

```
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00001089
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86431   0.00014  -0.00004   0.00064   0.00060
2.86491
    R2        2.66129  -0.00078  -0.00122  -0.00020  -0.00142
2.65986
    R3        2.63363  -0.00131  -0.00227   0.00001  -0.00227
2.63137
    R4        2.06566  -0.00015  -0.00034   0.00000  -0.00035
2.06531
    R5        2.96662  -0.00094  -0.00193  -0.00057  -0.00250
2.96412
    R6        2.86788  -0.00034  -0.00017  -0.00056  -0.00073
2.86715
    R7        2.90700  -0.00011  -0.00130   0.00015  -0.00115
2.90585
    R8        2.63823  -0.00130  -0.00232   0.00001  -0.00231
2.63591
    R9        2.06905  -0.00010  -0.00055   0.00014  -0.00041
2.06864
   R10        2.91674  -0.00068  -0.00205   0.00040  -0.00166
2.91507
   R11        2.87114  -0.00035   0.00036  -0.00064  -0.00029
2.87086
   R12        2.66194  -0.00080  -0.00103  -0.00028  -0.00131
2.66062
   R13        2.63504  -0.00120  -0.00213   0.00001  -0.00211
2.63293
   R14        2.90108  -0.00063  -0.00120  -0.00032  -0.00151
2.89957
   R15        2.63829  -0.00118  -0.00209   0.00002  -0.00207
2.63621
   R16        3.00838  -0.00141  -0.00268  -0.00131  -0.00400
3.00438
   R17        2.88985  -0.00080  -0.00113  -0.00069  -0.00182
2.88803
   R18        2.07018  -0.00011  -0.00052   0.00010  -0.00043
2.06975
   R19        2.88331  -0.00072  -0.00012  -0.00122  -0.00134
2.88197
   R20        2.05603  -0.00030  -0.00073   0.00002  -0.00071
2.05532
   R21        2.64825  -0.00123  -0.00224   0.00000  -0.00224
2.64601
   R22        2.05255  -0.00022  -0.00055   0.00002  -0.00053
2.05202
   R23        2.65011  -0.00124  -0.00226   0.00001  -0.00225
2.64787
   R24        2.05444  -0.00025  -0.00052  -0.00004  -0.00056
2.05388
```

This journal is © The Royal Society of Chemistry 2014

R25	2.64107	-0.00118	-0.00243	0.00019	-0.00224
2.63883					
R26	2.05425	-0.00024	-0.00051	-0.00004	-0.00055
2.05370					
R27	2.05679	-0.00031	-0.00070	-0.00002	-0.00071
2.05608					
R28	2.65023	-0.00130	-0.00253	0.00010	-0.00242
2.64781					
R29	2.05440	-0.00024	-0.00049	-0.00004	-0.00053
2.05387					
R30	2.63999	-0.00119	-0.00237	0.00012	-0.00224
2.63775					
R31	2.05461	-0.00025	-0.00050	-0.00005	-0.00055
2.05406					
R32	2.65231	-0.00134	-0.00259	0.00006	-0.00253
2.64978					
R33	2.05250	-0.00019	-0.00046	0.00000	-0.00046
2.05204					
R34	2.62469	-0.00013	-0.00025	-0.00003	-0.00027
2.62442					
R35	2.26733	-0.00135	-0.00208	0.00061	-0.00147
2.26586					
R36	2.63018	-0.00010	-0.00152	0.00070	-0.00081
2.62937					
R37	2.26759	-0.00119	-0.00128	0.00021	-0.00107
2.26653					
R38	2.07103	-0.00019	-0.00053	0.00003	-0.00050
2.07053					
R39	2.06446	-0.00001	-0.00057	0.00038	-0.00019
2.06427					
R40	2.07102	-0.00023	-0.00062	0.00003	-0.00059
2.07043					
A1	1.97972	-0.00010	-0.00025	0.00034	0.00010
1.97982					
A2	2.19515	0.00016	0.00071	-0.00036	0.00035
2.19550					
A3	2.10828	-0.00006	-0.00049	0.00002	-0.00047
2.10780					
A4	1.97288	0.00012	0.00144	0.00001	0.00146
1.97434					
A5	1.83088	0.00006	0.00167	-0.00021	0.00146
1.83234					
A6	1.87945	0.00005	0.00109	0.00004	0.00113
1.88058					
A7	1.93029	-0.00001	-0.00170	0.00016	-0.00153
1.92877					
A8	1.96628	0.00008	0.00019	0.00014	0.00034
1.96662					
A9	1.87658	-0.00032	-0.00278	-0.00018	-0.00296
1.87361					
A10	1.99484	0.00000	-0.00023	-0.00041	-0.00063
1.99420					

This journal is © The Royal Society of Chemistry 2014

A11	2.08467	0.00008	0.00047	0.00013	0.00060
2.08526					
A12	2.20368	-0.00008	-0.00024	0.00028	0.00003
2.20372					
A13	1.89993	0.00009	0.00127	-0.00075	0.00051
1.90044					
A14	1.91685	0.00000	-0.00024	-0.00020	-0.00043
1.91641					
A15	1.96574	-0.00024	-0.00432	0.00185	-0.00247
1.96327					
A16	1.96840	-0.00011	0.00022	0.00008	0.00030
1.96870					
A17	1.88341	0.00027	0.00304	-0.00051	0.00253
1.88594					
A18	1.82980	-0.00002	-0.00010	-0.00040	-0.00049
1.82931					
A19	1.98508	0.00005	-0.00021	0.00005	-0.00016
1.98492					
A20	2.19229	0.00000	0.00051	-0.00023	0.00029
2.19258					
A21	2.10580	-0.00005	-0.00033	0.00019	-0.00014
2.10566					
A22	1.98964	0.00001	-0.00034	0.00017	-0.00016
1.98948					
A23	2.08784	0.00005	0.00024	-0.00002	0.00022
2.08806					
A24	2.20563	-0.00006	0.00003	-0.00013	-0.00009
2.20554					
A25	1.85611	0.00013	0.00122	0.00040	0.00162
1.85772					
A26	1.81362	0.00008	0.00245	-0.00076	0.00168
1.81530					
A27	1.98464	0.00009	0.00078	0.00118	0.00197
1.98660					
A28	1.84553	-0.00015	-0.00282	0.00044	-0.00238
1.84315					
A29	1.99866	0.00001	-0.00003	-0.00029	-0.00031
1.99835					
A30	1.95029	-0.00016	-0.00154	-0.00101	-0.00255
1.94774					
A31	1.93542	0.00017	0.00044	0.00030	0.00075
1.93617					
A32	1.96326	-0.00011	0.00036	0.00045	0.00082
1.96408					
A33	1.81318	0.00023	0.00034	0.00047	0.00081
1.81399					
A34	1.88300	0.00006	0.00141	-0.00054	0.00086
1.88386					
A35	1.99544	-0.00068	-0.00568	-0.00060	-0.00628
1.98916					
A36	1.87413	0.00032	0.00305	-0.00004	0.00300
1.87713					

This journal is © The Royal Society of Chemistry 2014

A37	2.09644	0.00000	-0.00026	0.00015	-0.00011
2.09633					
A38	2.08572	-0.00007	-0.00014	-0.00010	-0.00024
2.08548					
A39	2.10102	0.00007	0.00040	-0.00005	0.00036
2.10137					
A40	2.10601	0.00003	-0.00053	0.00035	-0.00018
2.10583					
A41	2.08973	-0.00012	-0.00037	-0.00005	-0.00042
2.08931					
A42	2.08744	0.00010	0.00091	-0.00031	0.00060
2.08804					
A43	2.08711	-0.00007	-0.00017	-0.00005	-0.00022
2.08688					
A44	2.10197	0.00009	0.00024	0.00003	0.00027
2.10224					
A45	2.09410	-0.00003	-0.00007	0.00002	-0.00004
2.09405					
A46	2.09527	0.00010	0.00036	-0.00006	0.00029
2.09556					
A47	2.09187	-0.00006	-0.00026	0.00004	-0.00021
2.09166					
A48	2.09604	-0.00004	-0.00010	0.00002	-0.00007
2.09597					
A49	2.09736	-0.00001	-0.00038	0.00012	-0.00025
2.09711					
A50	2.08617	-0.00008	-0.00011	-0.00003	-0.00014
2.08603					
A51	2.09963	0.00009	0.00049	-0.00009	0.00040
2.10002					
A52	2.09296	-0.00007	-0.00031	0.00002	-0.00029
2.09266					
A53	2.09363	0.00010	0.00039	-0.00004	0.00036
2.09398					
A54	2.09660	-0.00003	-0.00008	0.00002	-0.00006
2.09654					
A55	2.09421	-0.00001	-0.00004	0.00010	0.00006
2.09427					
A56	2.10184	0.00010	0.00021	0.00001	0.00021
2.10206					
A57	2.08712	-0.00010	-0.00017	-0.00010	-0.00027
2.08685					
A58	2.09176	-0.00014	-0.00046	-0.00009	-0.00056
2.09120					
A59	2.10758	0.00002	-0.00070	0.00046	-0.00023
2.10735					
A60	2.08381	0.00012	0.00117	-0.00037	0.00080
2.08461					
A61	1.91538	-0.00004	-0.00023	0.00035	0.00018
1.91556					
A62	2.24794	-0.00034	-0.00164	0.00011	-0.00147
2.24647					

This journal is © The Royal Society of Chemistry 2014

A63	2.11984	0.00038	0.00173	-0.00047	0.00131	2.12115
A64	1.91962	-0.00005	0.00006	-0.00017	-0.00003	1.91959
A65	2.25625	-0.00042	-0.00153	-0.00014	-0.00159	2.25465
A66	2.10732	0.00047	0.00101	0.00030	0.00138	2.10870
A67	1.94647	-0.00011	0.00009	-0.00029	-0.00020	1.94627
A68	1.93308	-0.00003	-0.00087	0.00043	-0.00044	1.93265
A69	1.94424	-0.00036	-0.00238	0.00023	-0.00215	1.94209
A70	1.93291	-0.00008	-0.00004	-0.00012	-0.00016	1.93275
A71	1.87296	0.00017	0.00134	-0.00050	0.00085	1.87381
A72	1.88514	0.00010	-0.00008	0.00060	0.00052	1.88566
A73	1.89329	0.00023	0.00219	-0.00067	0.00152	1.89481
D1	3.12639	0.00008	0.00122	0.00002	0.00124	3.12763
D2	-1.05225	0.00018	0.00104	0.00010	0.00114	-1.05110
D3	0.94300	-0.00014	-0.00085	-0.00019	-0.00105	0.94195
D4	-0.02412	0.00003	-0.00143	0.00036	-0.00107	-0.02519
D5	2.08043	0.00013	-0.00160	0.00043	-0.00117	2.07925
D6	-2.20752	-0.00019	-0.00350	0.00014	-0.00336	-2.21088
D7	-0.00769	0.00000	0.00017	-0.00010	0.00007	-0.00762
D8	3.13499	-0.00008	-0.00185	-0.00091	-0.00276	3.13223
D9	-3.14086	0.00005	0.00266	-0.00041	0.00225	-3.13861
D10	0.00183	-0.00003	0.00063	-0.00122	-0.00058	0.00124
D11	0.01054	0.00003	0.00158	-0.00015	0.00143	0.01198
D12	-3.13850	0.00006	0.00225	0.00018	0.00243	-3.13607
D13	-3.14058	-0.00002	-0.00124	0.00021	-0.00103	3.14157
D14	-0.00644	0.00001	-0.00057	0.00054	-0.00003	-0.00647
D15	-1.13154	-0.00006	-0.00118	-0.00073	-0.00191	-1.13345

D16	1.03135	-0.00014	-0.00022	-0.00126	-0.00148	1.02987
D17	3.06362	-0.00030	-0.00310	-0.00076	-0.00387	3.05975
D18	1.00096	0.00012	0.00064	-0.00076	-0.00011	1.00085
D19	-3.11933	0.00004	0.00161	-0.00129	0.00032	-3.11901
D20	-1.08707	-0.00013	-0.00128	-0.00078	-0.00206	-1.08913
D21	-3.12880	0.00000	-0.00198	-0.00060	-0.00258	-3.13137
D22	-0.96590	-0.00008	-0.00102	-0.00113	-0.00215	-0.96805
D23	1.06636	-0.00025	-0.00391	-0.00062	-0.00453	1.06183
D24	-0.93617	0.00008	0.00126	0.00028	0.00153	-0.93463
D25	2.21005	0.00011	0.00530	-0.00144	0.00386	2.21391
D26	-3.12351	-0.00016	-0.00154	0.00014	-0.00141	-3.12492
D27	0.02271	-0.00012	0.00250	-0.00158	0.00092	0.02363
D28	1.02843	0.00002	0.00237	-0.00003	0.00234	1.03077
D29	-2.10854	0.00006	0.00641	-0.00175	0.00466	-2.10388
D30	-0.91643	0.00002	-0.00009	0.00039	0.00030	-0.91613
D31	1.02683	-0.00007	-0.00174	0.00072	-0.00102	1.02581
D32	-3.13211	-0.00017	-0.00155	-0.00036	-0.00192	-3.13403
D33	2.22398	0.00010	0.00209	0.00126	0.00336	2.22734
D34	-2.11594	0.00002	0.00044	0.00159	0.00203	-2.11391
D35	0.00831	-0.00008	0.00063	0.00051	0.00114	0.00944
D36	0.00417	0.00003	-0.00038	0.00102	0.00064	0.00481
D37	3.13710	0.00007	0.00060	0.00144	0.00204	3.13914
D38	-3.13619	-0.00006	-0.00267	0.00011	-0.00256	-3.13875
D39	-0.00326	-0.00002	-0.00168	0.00053	-0.00116	-0.00442
D40	-0.02674	0.00011	-0.00132	0.00177	0.00045	-0.02628
D41	-2.13716	-0.00002	-0.00370	0.00194	-0.00176	-2.13892

This journal is © The Royal Society of Chemistry 2014

D42	2.12479	-0.00048	-0.00768	0.00150	-0.00617	2.11862
D43	2.09569	0.00014	0.00029	0.00072	0.00101	2.09670
D44	-0.01473	0.00002	-0.00210	0.00089	-0.00121	-0.01594
D45	-2.03596	-0.00044	-0.00608	0.00045	-0.00562	-2.04159
D46	-2.14280	0.00040	0.00399	-0.00009	0.00390	-2.13891
D47	2.02995	0.00028	0.00161	0.00008	0.00169	2.03164
D48	0.00872	-0.00018	-0.00237	-0.00036	-0.00273	0.00599
D49	-2.07777	-0.00002	-0.00479	0.00091	-0.00388	-2.08165
D50	1.05528	0.00045	0.00883	-0.00079	0.00804	1.06332
D51	2.10785	-0.00016	-0.00572	0.00104	-0.00469	2.10316
D52	-1.04229	0.00031	0.00790	-0.00066	0.00724	-1.03505
D53	0.00581	-0.00016	-0.00745	0.00141	-0.00604	-0.00023
D54	3.13885	0.00031	0.00617	-0.00029	0.00589	-3.13844
D55	-0.00886	-0.00003	-0.00082	0.00019	-0.00062	-0.00949
D56	-3.13788	0.00002	0.00304	-0.00164	0.00139	-3.13648
D57	3.12836	-0.00006	-0.00463	0.00181	-0.00282	3.12554
D58	-0.00065	-0.00001	-0.00078	-0.00003	-0.00080	-0.00146
D59	0.00598	-0.00003	-0.00417	0.00187	-0.00230	0.00368
D60	-3.13905	0.00001	-0.00318	0.00231	-0.00087	-3.13992
D61	-3.13070	0.00001	0.00013	0.00004	0.00017	-3.13052
D62	0.00746	0.00004	0.00112	0.00049	0.00161	0.00906
D63	0.92333	0.00002	0.00045	-0.00014	0.00031	0.92365
D64	-0.99758	-0.00006	-0.00160	0.00037	-0.00124	-0.99882
D65	3.13059	0.00025	0.00242	0.00151	0.00393	3.13452
D66	-2.23184	-0.00003	-0.00371	0.00184	-0.00186	-2.23370
D67	2.13044	-0.00011	-0.00576	0.00235	-0.00342	2.12702

This journal is © The Royal Society of Chemistry 2014

D68	-0.02458	0.00020	-0.00174	0.00349	0.00175	-0.02283
D69	3.13083	0.00001	0.00062	0.00023	0.00084	3.13167
D70	-0.00660	-0.00004	-0.00026	-0.00045	-0.00071	-0.00730
D71	0.00351	0.00006	0.00499	-0.00186	0.00313	0.00664
D72	-3.13392	0.00001	0.00412	-0.00253	0.00158	-3.13234
D73	-0.96706	-0.00007	0.00188	-0.00191	-0.00003	-0.96709
D74	1.19014	-0.00006	0.00357	-0.00152	0.00206	1.19220
D75	-3.00970	-0.00004	0.00485	-0.00232	0.00253	-3.00717
D76	0.98391	0.00005	0.00314	-0.00161	0.00153	0.98544
D77	3.14111	0.00006	0.00483	-0.00121	0.00362	-3.13846
D78	-1.05874	0.00008	0.00611	-0.00202	0.00409	-1.05464
D79	-3.11401	-0.00014	0.00024	-0.00229	-0.00206	-3.11608
D80	-0.95681	-0.00013	0.00193	-0.00190	0.00002	-0.95679
D81	1.12653	-0.00010	0.00320	-0.00271	0.00050	1.12703
D82	-1.04223	0.00010	0.01298	-0.00008	0.01290	-1.02933
D83	-3.12548	0.00014	0.01343	0.00010	0.01353	-3.11195
D84	1.04889	0.00015	0.01228	0.00087	0.01316	1.06205
D85	3.10192	-0.00017	0.01069	-0.00136	0.00932	3.11124
D86	1.01866	-0.00012	0.01113	-0.00118	0.00995	1.02861
D87	-1.09015	-0.00011	0.00999	-0.00041	0.00958	-1.08057
D88	1.00419	0.00014	0.01557	-0.00097	0.01460	1.01879
D89	-1.07906	0.00019	0.01602	-0.00079	0.01523	-1.06383
D90	3.09531	0.00020	0.01487	-0.00001	0.01486	3.11017
D91	-0.02086	0.00047	0.01154	-0.00079	0.01075	-0.01011
D92	3.11976	-0.00045	-0.00915	-0.00323	-0.01237	3.10739
D93	2.09087	0.00045	0.00916	-0.00044	0.00871	2.09958

This journal is © The Royal Society of Chemistry 2014

D94	-1.05170	-0.00047	-0.01152	-0.00288	-0.01440	-1.06610
D95	-2.10399	0.00034	0.00954	-0.00152	0.00801	-2.09598
D96	1.03663	-0.00058	-0.01114	-0.00396	-0.01510	1.02153
D97	-0.00700	-0.00003	-0.00043	-0.00048	-0.00091	-0.00790
D98	3.13984	-0.00006	-0.00134	-0.00059	-0.00193	3.13791
D99	3.13115	0.00000	0.00056	-0.00003	0.00053	3.13168
D100	-0.00521	-0.00002	-0.00035	-0.00014	-0.00049	-0.00570
D101	-3.13946	0.00005	0.00120	0.00049	0.00168	-3.13778
D102	0.00707	0.00005	0.00095	0.00046	0.00141	0.00847
D103	0.00625	0.00001	0.00033	-0.00018	0.00015	0.00640
D104	-3.13041	0.00000	0.00008	-0.00021	-0.00012	-3.13053
D105	-0.00023	-0.00001	-0.00060	0.00001	-0.00060	-0.00083
D106	3.13611	0.00001	0.00031	0.00012	0.00043	3.13653
D107	-3.13687	-0.00002	-0.00085	-0.00002	-0.00087	-3.13775
D108	-0.00053	0.00001	0.00006	0.00009	0.00015	-0.00038
D109	-3.13301	-0.00001	-0.00033	-0.00019	-0.00052	-3.13353
D110	0.00504	0.00002	0.00027	0.00033	0.00060	0.00563
D111	0.00112	0.00001	0.00033	0.00014	0.00048	0.00160
D112	3.13917	0.00005	0.00093	0.00066	0.00159	3.14076
D113	-3.13772	-0.00004	-0.00049	-0.00069	-0.00118	-3.13890
D114	0.00093	-0.00002	-0.00002	-0.00052	-0.00054	0.00039
D115	0.00032	0.00000	0.00012	-0.00017	-0.00006	0.00026
D116	3.13897	0.00001	0.00058	0.00000	0.00058	3.13955
D117	-0.00556	0.00000	0.00008	-0.00017	-0.00008	-0.00564
D118	-3.13861	-0.00005	-0.00088	-0.00058	-0.00146	-3.14007
D119	3.13310	0.00001	0.00054	0.00001	0.00055	3.13366

This journal is © The Royal Society of Chemistry 2014

```
   D120        0.00006  -0.00003  -0.00042  -0.00041  -0.00083  -
0.00077
   D121       -0.01996   0.00048   0.01551  -0.00201   0.01350  -
0.00646
   D122        3.12944   0.00005   0.00306  -0.00046   0.00260
3.13204
   D123        0.02607  -0.00061  -0.01721   0.00177  -0.01544
0.01063
   D124       -3.11465   0.00022   0.00146   0.00396   0.00543  -
3.10922
         Item               Value     Threshold  Converged?
 Maximum Force            0.001415     0.000450     NO
 RMS     Force            0.000368     0.000300     NO
 Maximum Displacement     0.031377     0.001800     NO
 RMS     Displacement     0.005420     0.001200     NO
 Predicted change in Energy=-7.545439D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.707038   -0.047063   -0.893777
      2          6           0        0.299507   -0.056322   -1.456950
      3          1           0        0.273422    0.001659   -2.548016
      4          6           0        1.747884   -0.103507    0.512037
      5          6           0       -0.325983   -1.407393   -0.963285
      6          1           0        0.220149   -2.238674   -1.420485
      7          6           0       -0.471843    1.068763   -0.792731
      8          6           0       -0.434953    1.027492    0.614120
      9          6           0        0.365051   -0.151865    1.182847
     10          6           0       -0.310457   -1.457986    0.578397
     11          1           0        0.231945   -2.327718    0.964370
     12          6           0       -1.176400    2.071494   -1.455583
     13          1           0       -1.207639    2.089115   -2.542623
     14          6           0       -1.109291    2.001521    1.350754
     15          1           0       -1.099476    1.980238    2.436384
     16          6           0       -1.809048    3.015929    0.683933
     17          1           0       -2.330665    3.775694    1.260085
     18          6           0       -1.843921    3.052028   -0.711572
     19          1           0       -2.392368    3.838792   -1.222730
     20          6           0        2.882233   -0.002412   -1.639341
     21          1           0        2.839032    0.041043   -2.725643
     22          6           0        4.118633   -0.006014   -0.980133
     23          1           0        5.039622    0.036272   -1.555686
     24          6           0        4.165613   -0.060932    0.413831
     25          1           0        5.124562   -0.061208    0.925594
     26          6           0        2.981486   -0.113197    1.163021
     27          1           0        3.036929   -0.154092    2.246724
```

This journal is © The Royal Society of Chemistry 2014

28	6	0	-1.791173	-1.541870	-1.341543
29	6	0	-1.778554	-1.627212	0.955090
30	8	0	-2.563569	-1.658649	-0.193287
31	8	0	-2.273087	-1.748709	2.041012
32	8	0	-2.285262	-1.557544	-2.433939
33	6	0	0.420830	-0.202387	2.709271
34	1	0	0.978990	-1.082251	3.048099
35	1	0	-0.580773	-0.265761	3.140591
36	1	0	0.917034	0.688867	3.109072

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.516045	0.000000			
3	H	2.189552	1.092917	0.000000		
4	C	1.407540	2.444777	3.398386	0.000000	
5	C	2.447142	1.568546	2.203653	2.859654	0.000000
6	H	2.700263	2.184099	2.508636	3.259994	1.094678
7	C	2.450061	1.517229	2.185213	2.829103	2.486305
8	C	2.831351	2.450188	3.399006	2.460560	2.903231
9	C	2.474728	2.642339	3.735145	1.537710	2.580652
10	C	2.868499	2.545458	3.499420	2.464911	1.542591
11	H	3.290896	3.320632	4.214804	2.729431	2.207745
12	C	3.621895	2.589576	2.753110	4.141690	3.615000
13	H	3.972064	2.837794	2.559501	4.782641	3.936648
14	C	4.143227	3.755347	4.594753	3.646647	4.193930
15	H	4.803794	4.611158	5.535690	4.019024	4.861284
16	C	4.922799	4.297454	4.885489	4.734152	4.947585
17	H	5.962855	5.383720	5.960390	5.678234	5.985526
18	C	4.716659	3.848599	4.142514	4.935147	4.717408
19	H	5.658022	4.740566	4.856584	5.974347	5.644441
20	C	1.392459	2.589719	2.762536	2.434214	3.567026
21	H	2.155204	2.840466	2.572053	3.419660	3.901435
22	C	2.413489	3.849104	4.152585	2.802949	4.660338
23	H	3.398703	4.742047	4.868529	3.889802	5.587918
24	C	2.784712	4.294952	4.891381	2.420097	4.887110
25	H	3.871664	5.381235	5.966865	3.402172	5.923556
26	C	2.420539	3.749732	4.595498	1.394865	4.139502
27	H	3.412156	4.606542	5.536313	2.161789	4.814986
28	C	3.830460	2.567317	2.846158	4.246125	1.519193
29	C	4.250239	3.550208	4.374424	3.867006	2.416288
30	O	4.618006	3.515893	4.043499	4.637302	2.379667
31	O	5.229720	4.660274	5.532420	4.605720	3.596319
32	O	4.537853	3.144711	2.998498	5.201853	2.454413
33	C	3.828892	4.170546	5.263311	2.568791	3.936679
34	H	4.140055	4.670085	5.743622	2.825022	4.230824
35	H	4.643063	4.685739	5.758596	3.515433	4.267323
36	H	4.145901	4.667462	5.734905	2.839499	4.745892

		6	7	8	9	10
6	H	0.000000				
7	C	3.436869	0.000000			
8	C	3.903412	1.407940	0.000000		

This journal is © The Royal Society of Chemistry 2014

9	C	3.339627	2.468447	1.534386	0.000000	
10	C	2.210554	2.879323	2.488850	1.589850	0.000000
11	H	2.386546	3.888291	3.438730	2.190841	1.095267
12	C	4.530908	1.393285	2.433795	3.778983	4.164632
13	H	4.693350	2.155142	3.418935	4.623253	4.809119
14	C	5.237025	2.422996	1.395024	2.615138	3.633574
15	H	5.866521	3.413487	2.161009	2.874379	3.986985
16	C	6.013075	2.785698	2.418035	3.874344	4.719410
17	H	7.061497	3.872564	3.400531	4.764302	5.651314
18	C	5.723152	2.412991	2.800249	4.328199	4.935155
19	H	6.618153	3.397996	3.887017	5.414379	5.969444
20	C	3.483599	3.621324	4.140352	3.784612	4.150943
21	H	3.709326	3.969162	4.779757	4.629696	4.804482
22	C	4.514073	4.718339	4.934057	4.334643	4.914679
23	H	5.331133	5.659008	5.971729	5.420938	5.950669
24	C	4.865590	4.923210	4.731806	3.878650	4.691913
25	H	5.856510	5.962316	5.673666	4.767320	5.622363
26	C	4.337873	4.140951	3.643421	2.616796	3.603766
27	H	5.072292	4.800535	4.014411	2.875894	3.960864
28	C	2.130067	2.976111	3.502225	3.599162	2.426052
29	C	3.164183	3.468524	2.994825	2.612195	1.525071
30	O	3.097019	3.489044	3.521117	3.569448	2.390037
31	O	4.293978	4.383233	3.622437	3.200958	2.464889
32	O	2.787133	3.588808	4.404171	4.699068	3.603323
33	C	4.608864	3.831019	2.575776	1.528279	2.579135
34	H	4.677755	4.635057	3.517741	2.172948	2.811276
35	H	5.033615	4.154978	2.841975	2.177227	2.838892
36	H	5.438109	4.159010	2.857852	2.172984	3.538365

		11	12	13	14	15
11	H	0.000000				
12	C	5.214660	0.000000			
13	H	5.820637	1.087631	0.000000		
14	C	4.548683	2.808012	3.895604	0.000000	
15	H	4.743205	3.893797	4.981371	1.085882	0.000000
16	C	5.727029	2.422753	3.410475	1.401190	2.155744
17	H	6.626165	3.407563	4.308866	2.155845	2.474504
18	C	6.004970	1.400209	2.164441	2.428257	3.407720
19	H	7.049558	2.157809	2.491399	3.412429	4.302895
20	C	4.382965	4.561508	4.681608	5.374819	6.032946
21	H	5.101384	4.675412	4.539123	6.004144	6.776344
22	C	4.927244	5.707842	5.932968	6.065840	6.545719
23	H	5.920548	6.541489	6.649547	7.079458	7.576552
24	C	4.573309	6.048062	6.498858	5.740744	5.998187
25	H	5.392241	7.065447	7.533205	6.580010	6.722249
26	C	3.536035	5.377544	6.010885	4.608875	4.760060
27	H	3.773196	6.034273	6.781310	4.758210	4.658452
28	C	3.166671	3.667063	3.868741	4.502116	5.211183
29	C	2.129061	4.455823	5.135273	3.711087	3.958418
30	O	3.098826	4.175116	4.626409	4.230346	4.722312
31	O	2.787399	5.293661	6.072378	3.986866	3.929215
32	O	4.298605	3.918759	3.804104	5.326702	6.135310
33	C	2.756337	5.006764	5.956953	3.007332	2.673882

This journal is © The Royal Society of Chemistry 2014

34	H	2.539919	5.905503	6.789336	4.092865	3.751407
35	H	3.106142	5.190602	6.183634	2.936565	2.410284
36	H	3.764157	5.208665	6.198111	2.986759	2.487259
		16	17	18	19	20
16	C	0.000000				
17	H	1.086867	0.000000			
18	C	1.396407	2.155932	0.000000		
19	H	2.157019	2.484384	1.086773	0.000000	
20	C	6.042855	7.060812	5.703235	6.538335	0.000000
21	H	6.486895	7.520599	5.920520	6.636956	1.088029
22	C	6.858473	7.804700	6.706399	7.565350	1.401161
23	H	7.797341	8.731150	7.562438	8.354908	2.159356
24	C	6.725816	7.591935	6.860871	7.803415	2.421983
25	H	7.589606	8.391311	7.805914	8.736677	3.407402
26	C	5.741965	6.584211	6.067726	7.084372	2.806307
27	H	5.997903	6.725157	6.546251	7.580072	3.892099
28	C	4.987626	5.944410	4.637192	5.415448	4.929437
29	C	4.651153	5.439600	4.967628	5.915815	5.576198
30	O	4.815652	5.630153	4.793432	5.595616	5.872900
31	O	4.975819	5.579623	5.550493	6.471971	6.570531
32	O	5.555589	6.487782	4.940596	5.531630	5.454616
33	C	4.408164	5.049356	5.236648	6.301257	5.000892
34	H	5.491586	6.144139	6.260688	7.336396	5.173053
35	H	4.279406	4.788714	5.238552	6.258419	5.908428
36	H	4.327590	4.847143	5.273018	6.295925	5.185296
		21	22	23	24	25
21	H	0.000000				
22	C	2.164809	0.000000			
23	H	2.492271	1.086863	0.000000		
24	C	3.409767	1.395836	2.156928	0.000000	
25	H	4.308786	2.155629	2.484647	1.086961	0.000000
26	C	3.894328	2.428518	3.413156	1.402203	2.156814
27	H	4.980127	3.406554	4.301783	2.154554	2.472291
28	C	5.085287	6.116803	7.013997	6.384185	7.426955
29	C	6.136202	6.414840	7.453770	6.170844	7.078576
30	O	6.204021	6.928358	7.908059	6.942851	7.931649
31	O	7.215121	7.281372	8.342548	6.852238	7.669226
32	O	5.375776	6.747642	7.547549	7.208567	8.272302
33	C	5.953591	5.227237	6.291268	4.394594	5.032547
34	H	6.169087	5.219415	6.239765	4.258759	4.767947
35	H	6.797198	6.255577	7.330422	5.477714	6.123634
36	H	6.177187	5.239722	6.259519	4.287165	4.799320
		26	27	28	29	30
26	C	0.000000				
27	H	1.085890	0.000000			
28	C	5.576041	6.173504	0.000000		
29	C	4.999345	5.198776	2.298254	0.000000	
30	O	5.914019	6.291495	1.388785	1.391405	0.000000
31	O	5.572818	5.548097	3.422967	1.199395	2.254902
32	O	6.539335	7.225233	1.199041	3.427409	2.260132
33	C	2.992625	2.657114	4.805859	3.153501	4.410463
34	H	2.915918	2.395578	5.210951	3.504527	4.836170

This journal is © The Royal Society of Chemistry 2014

35	H	4.077223	3.728168	4.814879	2.839832	4.121452
36	H	2.948285	2.438889	5.667323	4.155725	5.341442

		31	32	33	34	35
31	O	0.000000				
32	O	4.479049	0.000000			
33	C	3.177243	5.967579	0.000000		
34	H	3.469062	6.397967	1.095677	0.000000	
35	H	2.504424	5.970710	1.092365	1.762972	0.000000
36	H	4.154444	6.784249	1.095624	1.773250	1.776438

		36
36	H	0.000000

Stoichiometry C19H14O3
Framework group C1[X(C19H14O3)]
Deg. of freedom 102
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.707407	-0.052173	-0.893866
2	6	0	0.299927	-0.045538	-1.457201
3	1	0	0.274500	0.019546	-2.547882
4	6	0	1.747565	-0.117833	0.511567
5	6	0	-0.337454	-1.394158	-0.972115
6	1	0	0.201430	-2.227297	-1.434503
7	6	0	-0.461619	1.082058	-0.785965
8	6	0	-0.425285	1.031598	0.620602
9	6	0	0.364269	-0.158291	1.181946
10	6	0	-0.322583	-1.454602	0.569219
11	1	0	0.212120	-2.331473	0.949745
12	6	0	-1.157266	2.095088	-1.442539
13	1	0	-1.188201	2.119835	-2.529448
14	6	0	-1.091156	2.006840	1.363307
15	1	0	-1.081676	1.978628	2.448782
16	6	0	-1.781900	3.031529	0.702838
17	1	0	-2.296914	3.792192	1.283727
18	6	0	-1.816265	3.076728	-0.692414
19	1	0	-2.357723	3.871478	-1.198647
20	6	0	2.883051	-0.013130	-1.639039
21	1	0	2.840380	0.037549	-2.725049
22	6	0	4.119281	-0.031730	-0.979766
23	1	0	5.040684	0.006105	-1.554967
24	6	0	4.165587	-0.095844	0.413828
25	1	0	5.124427	-0.107755	0.925657
26	6	0	2.980946	-0.142444	1.162577
27	1	0	3.035880	-0.190655	2.246005
28	6	0	-1.803716	-1.513393	-1.351333
29	6	0	-1.792158	-1.613319	0.944719
30	8	0	-2.577262	-1.630630	-0.203898

```
     31          8           0       -2.287886   -1.737317    2.029812
     32          8           0       -2.297774   -1.517847   -2.443846
     33          6           0        0.419395   -0.218921    2.708026
     34          1           0        0.969772   -1.105765    3.041345
     35          1           0       -0.582784   -0.276227    3.138857
     36          1           0        0.923340    0.665409    3.113478
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.4234843      0.2801880
0.2680395
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   446 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   446 basis functions,   760 primitive gaussians,   446 cartesian
basis functions
    76 alpha electrons       76 beta electrons
       nuclear repulsion energy      1805.7418845387 Hartrees.
 NAtoms=   36 NActive=   36 NUniq=   36 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   446 RedAO= T  NBF=   446
 NBsUse=   441 1.00D-06 NBFU=   441
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -958.192621341     A.U. after   12 cycles
             Convg  =    0.7988D-08             -V/T =  2.0094
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000104164    0.000021828    0.000068925
      2        6          -0.000094427   -0.000051488    0.000015832
      3        1           0.000010935   -0.000003704    0.000016738
      4        6           0.000119526    0.000028730   -0.000035201
      5        6          -0.000022810   -0.000022787   -0.000105684
      6        1           0.000012176   -0.000012530    0.000016430
      7        6          -0.000029470    0.000042160    0.000037773
      8        6           0.000001691    0.000039007   -0.000014393
      9        6          -0.000068224   -0.000042448   -0.000008472
     10        6          -0.000083762    0.000012158    0.000036874
```

```
     11        1          -0.000000793    0.000024446    0.000002147
     12        6          -0.000000364    0.000047304    0.000062418
     13        1          -0.000004345   -0.000001306    0.000025512
     14        6           0.000007528    0.000026062   -0.000044070
     15        1          -0.000012422   -0.000001822   -0.000013730
     16        6           0.000034267   -0.000062906   -0.000038212
     17        1           0.000014768   -0.000007886   -0.000005011
     18        6           0.000037210   -0.000073248    0.000033404
     19        1           0.000016307   -0.000001724    0.000015695
     20        6           0.000004676   -0.000004424    0.000054144
     21        1           0.000004523   -0.000007314    0.000023500
     22        6          -0.000072217   -0.000017557    0.000040627
     23        1          -0.000015077    0.000003637    0.000008814
     24        6          -0.000074851   -0.000012532   -0.000054569
     25        1          -0.000017126   -0.000008429   -0.000003064
     26        6          -0.000036218    0.000009401   -0.000066134
     27        1          -0.000019894   -0.000000081    0.000001934
     28        6          -0.000027244    0.000213588    0.000134171
     29        6           0.000132033   -0.000198935    0.000078626
     30        8          -0.000057260    0.000028001   -0.000130018
     31        8           0.000027711    0.000095010   -0.000115518
     32        8           0.000047330   -0.000076914    0.000008755
     33        6           0.000055244    0.000029612   -0.000044197
     34        1          -0.000015767    0.000010366    0.000005785
     35        1           0.000015380   -0.000007000   -0.000024878
     36        1           0.000006800   -0.000016275    0.000015051
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000213588 RMS     0.000054262


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000144703 RMS     0.000029820
 Search for a local minimum.
 Step number   4 out of a maximum of  216
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
 DE= -7.48D-05 DEPred=-7.55D-05 R= 9.91D-01
 SS=  1.41D+00  RLast= 6.02D-02 DXNew= 2.5227D-01 1.8069D-01
 Trust test= 9.91D-01 RLast= 6.02D-02 DXMaxT set to 1.81D-01
     Eigenvalues ---    0.00403   0.00429   0.00799   0.01090
0.01141
     Eigenvalues ---    0.01161   0.01427   0.01486   0.01561
0.01786
     Eigenvalues ---    0.02112   0.02117   0.02127   0.02130
0.02131
     Eigenvalues ---    0.02134   0.02140   0.02145   0.02151
0.02157
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02160   0.02166   0.02752   0.03392
0.03896
     Eigenvalues ---    0.04191   0.04600   0.05183   0.05241
0.05346
     Eigenvalues ---    0.05473   0.05530   0.05604   0.05895
0.06440
     Eigenvalues ---    0.08142   0.08537   0.09313   0.10158
0.12682
     Eigenvalues ---    0.15856   0.15996   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16028   0.16451   0.20315   0.21740
0.22000
     Eigenvalues ---    0.22001   0.22430   0.22614   0.22631
0.24530
     Eigenvalues ---    0.24569   0.24594   0.24920   0.25146
0.26366
     Eigenvalues ---    0.27479   0.27734   0.28804   0.28980
0.29718
     Eigenvalues ---    0.29842   0.30139   0.34210   0.34229
0.34258
     Eigenvalues ---    0.34323   0.34504   0.34583   0.35107
0.35153
     Eigenvalues ---    0.35209   0.35218   0.35225   0.35260
0.35336
     Eigenvalues ---    0.35358   0.36665   0.39880   0.41996
0.42042
     Eigenvalues ---    0.43364   0.44070   0.44791   0.45815
0.46021
     Eigenvalues ---    0.46140   0.46344   0.46368   0.46851
0.47693
     Eigenvalues ---    1.03955
1.057421000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     4    3    2    1
 RFO step:  Lambda=-5.07455215D-07.
 DIIS coeffs:      0.70301      0.10849      0.07779      0.11071
 Iteration  1 RMS(Cart)=  0.00048209 RMS(Int)=  0.00000301
 Iteration  2 RMS(Cart)=  0.00000053 RMS(Int)=  0.00000297
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86491   0.00003  -0.00019   0.00025   0.00006
2.86497
    R2        2.65986  -0.00009   0.00001  -0.00023  -0.00022
2.65965
    R3        2.63137  -0.00009  -0.00008  -0.00010  -0.00019
2.63118
    R4        2.06531  -0.00002  -0.00001  -0.00003  -0.00004
2.06527
```

This journal is © The Royal Society of Chemistry 2014

R5	2.96412	-0.00007	0.00010	-0.00034	-0.00024
2.96388					
R6	2.86715	0.00000	0.00016	-0.00013	0.00003
2.86718					
R7	2.90585	-0.00003	-0.00009	-0.00004	-0.00013
2.90572					
R8	2.63591	-0.00014	-0.00009	-0.00019	-0.00027
2.63564					
R9	2.06864	0.00001	-0.00006	0.00008	0.00001
2.06866					
R10	2.91507	-0.00003	-0.00019	0.00016	-0.00003
2.91505					
R11	2.87086	-0.00007	0.00020	-0.00037	-0.00017
2.87069					
R12	2.66062	-0.00007	0.00004	-0.00017	-0.00013
2.66049					
R13	2.63293	-0.00006	-0.00008	-0.00006	-0.00014
2.63279					
R14	2.89957	-0.00004	0.00005	-0.00022	-0.00017
2.89940					
R15	2.63621	-0.00007	-0.00008	-0.00006	-0.00015
2.63607					
R16	3.00438	0.00000	0.00028	-0.00033	-0.00005
3.00433					
R17	2.88803	-0.00004	0.00016	-0.00030	-0.00014
2.88789					
R18	2.06975	-0.00002	-0.00005	0.00000	-0.00004
2.06971					
R19	2.88197	-0.00009	0.00035	-0.00058	-0.00023
2.88174					
R20	2.05532	-0.00002	-0.00003	-0.00003	-0.00006
2.05526					
R21	2.64601	-0.00010	-0.00008	-0.00012	-0.00020
2.64581					
R22	2.05202	-0.00002	-0.00003	-0.00002	-0.00004
2.05198					
R23	2.64787	-0.00010	-0.00009	-0.00012	-0.00020
2.64766					
R24	2.05388	-0.00002	-0.00001	-0.00004	-0.00004
2.05384					
R25	2.63883	-0.00009	-0.00014	-0.00004	-0.00019
2.63864					
R26	2.05370	-0.00002	-0.00001	-0.00004	-0.00004
2.05366					
R27	2.05608	-0.00002	-0.00002	-0.00004	-0.00006
2.05601					
R28	2.64781	-0.00010	-0.00012	-0.00008	-0.00020
2.64761					
R29	2.05387	-0.00002	0.00000	-0.00004	-0.00004
2.05383					
R30	2.63775	-0.00008	-0.00012	-0.00005	-0.00017
2.63758					

This journal is © The Royal Society of Chemistry 2014

R31	2.05406	-0.00002	0.00000	-0.00004	-0.00004
2.05401					
R32	2.64978	-0.00009	-0.00011	-0.00008	-0.00019
2.64959					
R33	2.05204	0.00000	-0.00002	0.00001	-0.00001
2.05203					
R34	2.62442	-0.00009	0.00000	-0.00015	-0.00015
2.62427					
R35	2.26586	-0.00003	-0.00025	0.00020	-0.00005
2.26581					
R36	2.62937	0.00007	-0.00026	0.00034	0.00008
2.62946					
R37	2.26653	-0.00012	-0.00011	0.00000	-0.00011
2.26642					
R38	2.07053	-0.00002	-0.00003	-0.00002	-0.00004
2.07048					
R39	2.06427	-0.00002	-0.00013	0.00007	-0.00006
2.06421					
R40	2.07043	0.00000	-0.00003	0.00002	-0.00001
2.07041					
A1	1.97982	0.00000	-0.00011	0.00009	-0.00002
1.97980					
A2	2.19550	0.00000	0.00013	-0.00010	0.00003
2.19553					
A3	2.10780	0.00000	-0.00002	0.00002	-0.00001
2.10780					
A4	1.97434	0.00000	0.00005	-0.00009	-0.00004
1.97430					
A5	1.83234	0.00001	0.00013	0.00003	0.00016
1.83250					
A6	1.88058	-0.00002	0.00003	-0.00003	0.00000
1.88058					
A7	1.92877	-0.00001	-0.00011	0.00004	-0.00008
1.92869					
A8	1.96662	0.00001	-0.00004	0.00009	0.00005
1.96667					
A9	1.87361	0.00001	-0.00005	-0.00004	-0.00009
1.87352					
A10	1.99420	0.00000	0.00011	-0.00012	-0.00001
1.99420					
A11	2.08526	0.00003	-0.00002	0.00012	0.00010
2.08536					
A12	2.20372	-0.00003	-0.00009	0.00000	-0.00009
2.20363					
A13	1.90044	0.00001	0.00027	-0.00001	0.00026
1.90070					
A14	1.91641	0.00000	0.00005	-0.00011	-0.00007
1.91635					
A15	1.96327	-0.00003	-0.00070	0.00022	-0.00047
1.96280					
A16	1.96870	-0.00002	-0.00001	-0.00008	-0.00008
1.96862					

This journal is © The Royal Society of Chemistry 2014

A17	1.88594	0.00002	0.00025	0.00010	0.00035
1.88629					
A18	1.82931	0.00001	0.00011	-0.00012	-0.00001
1.82930					
A19	1.98492	-0.00001	-0.00002	0.00001	-0.00001
1.98491					
A20	2.19258	0.00002	0.00008	-0.00004	0.00005
2.19263					
A21	2.10566	-0.00001	-0.00007	0.00003	-0.00004
2.10563					
A22	1.98948	0.00001	-0.00006	0.00002	-0.00004
1.98944					
A23	2.08806	0.00000	0.00001	0.00003	0.00005
2.08811					
A24	2.20554	-0.00001	0.00004	-0.00004	-0.00001
2.20553					
A25	1.85772	0.00000	-0.00007	0.00002	-0.00005
1.85767					
A26	1.81530	0.00001	0.00031	-0.00024	0.00007
1.81537					
A27	1.98660	-0.00003	-0.00031	0.00004	-0.00027
1.98633					
A28	1.84315	0.00000	-0.00023	0.00034	0.00011
1.84326					
A29	1.99835	-0.00001	0.00008	-0.00008	0.00000
1.99835					
A30	1.94774	0.00002	0.00023	-0.00007	0.00017
1.94791					
A31	1.93617	-0.00001	-0.00007	0.00007	0.00000
1.93617					
A32	1.96408	0.00001	-0.00011	0.00019	0.00009
1.96416					
A33	1.81399	-0.00002	-0.00013	0.00006	-0.00006
1.81393					
A34	1.88386	-0.00001	0.00021	-0.00036	-0.00015
1.88371					
A35	1.98916	0.00002	-0.00003	0.00012	0.00009
1.98925					
A36	1.87713	0.00000	0.00011	-0.00006	0.00005
1.87718					
A37	2.09633	0.00000	-0.00005	0.00005	0.00000
2.09633					
A38	2.08548	0.00000	0.00002	-0.00004	-0.00002
2.08546					
A39	2.10137	0.00000	0.00003	-0.00001	0.00002
2.10139					
A40	2.10583	0.00001	-0.00012	0.00017	0.00005
2.10588					
A41	2.08931	-0.00001	0.00000	-0.00005	-0.00005
2.08926					
A42	2.08804	0.00000	0.00012	-0.00012	0.00000
2.08804					

This journal is © The Royal Society of Chemistry 2014

A43	2.08688	0.00000	0.00001	-0.00002	-0.00001
2.08687					
A44	2.10224	0.00001	0.00000	0.00003	0.00003
2.10226					
A45	2.09405	0.00000	-0.00001	0.00000	-0.00001
2.09404					
A46	2.09556	0.00001	0.00003	0.00000	0.00004
2.09559					
A47	2.09166	0.00000	-0.00002	0.00002	0.00000
2.09166					
A48	2.09597	-0.00001	-0.00001	-0.00003	-0.00004
2.09593					
A49	2.09711	0.00001	-0.00005	0.00009	0.00004
2.09715					
A50	2.08603	-0.00002	0.00000	-0.00006	-0.00006
2.08598					
A51	2.10002	0.00001	0.00005	-0.00002	0.00002
2.10004					
A52	2.09266	0.00000	-0.00002	-0.00001	-0.00002
2.09264					
A53	2.09398	0.00000	0.00002	0.00000	0.00003
2.09401					
A54	2.09654	0.00000	-0.00001	0.00001	0.00000
2.09653					
A55	2.09427	0.00000	-0.00003	0.00004	0.00001
2.09428					
A56	2.10206	0.00001	0.00001	0.00003	0.00003
2.10209					
A57	2.08685	-0.00001	0.00002	-0.00006	-0.00004
2.08682					
A58	2.09120	-0.00002	0.00001	-0.00010	-0.00009
2.09111					
A59	2.10735	-0.00001	-0.00016	0.00011	-0.00005
2.10729					
A60	2.08461	0.00003	0.00015	0.00000	0.00015
2.08476					
A61	1.91556	0.00004	-0.00013	0.00024	0.00013
1.91569					
A62	2.24647	-0.00005	-0.00011	-0.00011	-0.00020
2.24626					
A63	2.12115	0.00001	0.00019	-0.00014	0.00005
2.12121					
A64	1.91959	0.00002	0.00003	0.00007	0.00012
1.91971					
A65	2.25465	0.00000	-0.00003	0.00000	-0.00001
2.25464					
A66	2.10870	-0.00003	-0.00006	-0.00001	-0.00004
2.10866					
A67	1.94627	-0.00006	0.00008	-0.00026	-0.00018
1.94609					
A68	1.93265	0.00002	-0.00016	0.00021	0.00006
1.93270					

A69	1.94209	-0.00003	-0.00015	-0.00004	-0.00020	1.94190
A70	1.93275	0.00003	0.00003	0.00011	0.00015	1.93290
A71	1.87381	0.00000	0.00019	-0.00023	-0.00003	1.87378
A72	1.88566	-0.00002	-0.00018	0.00013	-0.00004	1.88561
A73	1.89481	0.00000	0.00027	-0.00020	0.00007	1.89488
D1	3.12763	0.00000	0.00003	-0.00029	-0.00025	3.12738
D2	-1.05110	-0.00001	0.00001	-0.00027	-0.00026	-1.05137
D3	0.94195	0.00000	0.00002	-0.00031	-0.00029	0.94166
D4	-0.02519	0.00000	-0.00016	-0.00017	-0.00033	-0.02552
D5	2.07925	-0.00002	-0.00018	-0.00016	-0.00034	2.07892
D6	-2.21088	-0.00001	-0.00017	-0.00020	-0.00037	-2.21125
D7	-0.00762	0.00000	0.00004	0.00040	0.00045	-0.00718
D8	3.13223	0.00000	0.00020	-0.00004	0.00016	3.13239
D9	-3.13861	0.00000	0.00022	0.00030	0.00052	-3.13810
D10	0.00124	0.00000	0.00038	-0.00015	0.00023	0.00147
D11	0.01198	0.00000	0.00010	-0.00019	-0.00009	0.01189
D12	-3.13607	0.00000	0.00003	-0.00003	-0.00001	-3.13607
D13	3.14157	0.00000	-0.00010	-0.00006	-0.00017	3.14141
D14	-0.00647	0.00000	-0.00018	0.00009	-0.00008	-0.00656
D15	-1.13345	0.00001	0.00014	-0.00055	-0.00041	-1.13386
D16	1.02987	0.00000	0.00034	-0.00072	-0.00038	1.02949
D17	3.05975	-0.00001	0.00009	-0.00081	-0.00073	3.05903
D18	1.00085	0.00001	0.00022	-0.00062	-0.00040	1.00045
D19	-3.11901	-0.00001	0.00042	-0.00079	-0.00037	-3.11938
D20	-1.08913	-0.00001	0.00016	-0.00088	-0.00071	-1.08985
D21	-3.13137	0.00002	0.00007	-0.00051	-0.00044	-3.13182

This journal is © The Royal Society of Chemistry 2014

D22	-0.96805	0.00001	0.00027	-0.00068	-0.00042	-0.96846
D23	1.06183	0.00000	0.00002	-0.00078	-0.00076	1.06107
D24	-0.93463	0.00001	-0.00004	0.00003	-0.00001	-0.93465
D25	2.21391	0.00000	0.00061	-0.00047	0.00014	2.21404
D26	-3.12492	0.00001	-0.00010	0.00010	0.00000	-3.12491
D27	0.02363	0.00001	0.00055	-0.00040	0.00015	0.02378
D28	1.03077	0.00001	0.00010	0.00003	0.00013	1.03090
D29	-2.10388	0.00001	0.00075	-0.00047	0.00028	-2.10360
D30	-0.91613	-0.00001	-0.00012	-0.00030	-0.00043	-0.91656
D31	1.02581	-0.00001	-0.00028	-0.00002	-0.00030	1.02551
D32	-3.13403	0.00001	0.00004	-0.00024	-0.00020	-3.13423
D33	2.22734	-0.00001	-0.00029	0.00018	-0.00011	2.22722
D34	-2.11391	-0.00001	-0.00044	0.00046	0.00001	-2.11390
D35	0.00944	0.00001	-0.00012	0.00024	0.00011	0.00956
D36	0.00481	-0.00001	-0.00031	0.00008	-0.00023	0.00458
D37	3.13914	0.00000	-0.00039	0.00034	-0.00006	3.13909
D38	-3.13875	-0.00001	-0.00013	-0.00043	-0.00056	-3.13931
D39	-0.00442	0.00000	-0.00022	-0.00016	-0.00038	-0.00480
D40	-0.02628	-0.00001	-0.00054	0.00108	0.00054	-0.02575
D41	-2.13892	0.00000	-0.00068	0.00135	0.00067	-2.13825
D42	2.11862	0.00000	-0.00069	0.00129	0.00060	2.11922
D43	2.09670	0.00000	-0.00017	0.00094	0.00077	2.09747
D44	-0.01594	0.00001	-0.00031	0.00121	0.00090	-0.01504
D45	-2.04159	0.00001	-0.00032	0.00115	0.00083	-2.04075
D46	-2.13891	0.00002	0.00020	0.00094	0.00114	-2.13777
D47	2.03164	0.00003	0.00005	0.00122	0.00127	2.03291

This journal is © The Royal Society of Chemistry 2014

D48	0.00599	0.00003	0.00005	0.00116	0.00121	0.00720
D49	-2.08165	-0.00001	-0.00023	-0.00052	-0.00075	-2.08239
D50	1.06332	0.00004	0.00011	0.00388	0.00398	1.06731
D51	2.10316	-0.00003	-0.00029	-0.00072	-0.00101	2.10215
D52	-1.03505	0.00003	0.00004	0.00368	0.00372	-1.03133
D53	-0.00023	-0.00002	-0.00047	-0.00061	-0.00109	-0.00131
D54	-3.13844	0.00003	-0.00014	0.00378	0.00364	-3.13480
D55	-0.00949	0.00000	-0.00008	0.00015	0.00008	-0.00941
D56	-3.13648	0.00000	0.00059	-0.00041	0.00018	-3.13631
D57	3.12554	0.00000	-0.00069	0.00063	-0.00006	3.12548
D58	-0.00146	0.00000	-0.00002	0.00006	0.00004	-0.00142
D59	0.00368	0.00000	-0.00070	0.00068	-0.00001	0.00366
D60	-3.13992	0.00000	-0.00079	0.00054	-0.00025	-3.14017
D61	-3.13052	0.00000	-0.00001	0.00015	0.00014	-3.13038
D62	0.00906	-0.00001	-0.00010	0.00001	-0.00009	0.00897
D63	0.92365	0.00001	0.00005	0.00006	0.00011	0.92375
D64	-0.99882	0.00000	-0.00017	0.00018	0.00001	-0.99881
D65	3.13452	-0.00002	-0.00035	0.00007	-0.00028	3.13423
D66	-2.23370	0.00001	-0.00067	0.00067	0.00000	-2.23370
D67	2.12702	0.00000	-0.00089	0.00079	-0.00010	2.12692
D68	-0.02283	-0.00002	-0.00107	0.00068	-0.00039	-0.02322
D69	3.13167	-0.00001	-0.00004	-0.00014	-0.00018	3.13149
D70	-0.00730	0.00000	0.00012	-0.00009	0.00004	-0.00727
D71	0.00664	-0.00001	0.00072	-0.00079	-0.00007	0.00657
D72	-3.13234	0.00000	0.00088	-0.00073	0.00015	-3.13218
D73	-0.96709	0.00000	0.00061	-0.00093	-0.00033	-0.96741

This journal is © The Royal Society of Chemistry 2014

D74	1.19220	0.00000	0.00057	-0.00089	-0.00032	1.19188
D75	-3.00717	0.00002	0.00083	-0.00114	-0.00030	-3.00747
D76	0.98544	0.00001	0.00057	-0.00088	-0.00031	0.98512
D77	-3.13846	0.00001	0.00053	-0.00084	-0.00031	-3.13877
D78	-1.05464	0.00002	0.00079	-0.00109	-0.00029	-1.05493
D79	-3.11608	0.00001	0.00066	-0.00079	-0.00014	-3.11621
D80	-0.95679	0.00001	0.00062	-0.00075	-0.00013	-0.95692
D81	1.12703	0.00003	0.00088	-0.00100	-0.00011	1.12692
D82	-1.02933	-0.00002	0.00050	-0.00080	-0.00030	-1.02963
D83	-3.11195	-0.00001	0.00046	-0.00063	-0.00017	-3.11212
D84	1.06205	-0.00001	0.00019	-0.00042	-0.00022	1.06183
D85	3.11124	0.00000	0.00078	-0.00079	-0.00001	3.11123
D86	1.02861	0.00001	0.00075	-0.00062	0.00012	1.02874
D87	-1.08057	0.00001	0.00048	-0.00041	0.00007	-1.08050
D88	1.01879	-0.00001	0.00085	-0.00113	-0.00028	1.01851
D89	-1.06383	0.00000	0.00081	-0.00096	-0.00014	-1.06397
D90	3.11017	0.00000	0.00055	-0.00075	-0.00020	3.10997
D91	-0.01011	-0.00003	0.00039	-0.00139	-0.00100	-0.01111
D92	3.10739	0.00004	0.00120	0.00172	0.00293	3.11031
D93	2.09958	-0.00004	0.00020	-0.00119	-0.00099	2.09859
D94	-1.06610	0.00003	0.00102	0.00192	0.00293	-1.06317
D95	-2.09598	-0.00003	0.00052	-0.00161	-0.00109	-2.09707
D96	1.02153	0.00004	0.00134	0.00150	0.00284	1.02436
D97	-0.00790	0.00000	0.00012	-0.00005	0.00008	-0.00782
D98	3.13791	0.00000	0.00012	-0.00015	-0.00002	3.13788
D99	3.13168	0.00000	0.00003	-0.00019	-0.00016	3.13152

```
   D100      -0.00570  -0.00001   0.00003  -0.00029  -0.00026  -
0.00596
   D101      -3.13778   0.00000  -0.00010   0.00011   0.00001  -
3.13777
   D102       0.00847   0.00000  -0.00010   0.00005  -0.00005
0.00842
   D103       0.00640   0.00001   0.00006   0.00017   0.00023
0.00663
   D104      -3.13053   0.00000   0.00006   0.00010   0.00016  -
3.13037
   D105      -0.00083   0.00000  -0.00002   0.00002   0.00000  -
0.00084
   D106       3.13653   0.00000  -0.00002   0.00012   0.00010
3.13663
   D107      -3.13775   0.00000  -0.00003  -0.00004  -0.00007  -
3.13782
   D108      -0.00038   0.00000  -0.00003   0.00006   0.00003  -
0.00035
   D109      -3.13353   0.00000   0.00004   0.00004   0.00008  -
3.13345
   D110       0.00563   0.00000  -0.00009   0.00004  -0.00005
0.00559
   D111       0.00160   0.00001  -0.00003   0.00020   0.00017
0.00176
   D112       3.14076   0.00000  -0.00016   0.00019   0.00003
3.14080
   D113      -3.13890   0.00000   0.00018  -0.00015   0.00003  -
3.13887
   D114       0.00039   0.00000   0.00015  -0.00011   0.00004
0.00043
   D115       0.00026   0.00000   0.00005  -0.00016  -0.00010
0.00016
   D116       3.13955   0.00000   0.00002  -0.00011  -0.00009
3.13946
   D117      -0.00564   0.00000   0.00005   0.00005   0.00010  -
0.00554
   D118      -3.14007   0.00000   0.00014  -0.00021  -0.00007  -
3.14014
   D119       3.13366   0.00000   0.00002   0.00009   0.00011
3.13377
   D120      -0.00077   0.00000   0.00010  -0.00016  -0.00006  -
0.00083
   D121      -0.00646   0.00000   0.00075  -0.00027   0.00049  -
0.00598
   D122       3.13204  -0.00005   0.00045  -0.00429  -0.00385
3.12819
   D123       0.01063   0.00002  -0.00072   0.00107   0.00035
0.01098
   D124      -3.10922  -0.00005  -0.00146  -0.00173  -0.00319  -
3.11241
         Item               Value     Threshold  Converged?
 Maximum Force            0.000145     0.000450     YES
```

This journal is © The Royal Society of Chemistry 2014

```
 RMS     Force            0.000030     0.000300     YES
 Maximum Displacement     0.003325     0.001800     NO
 RMS     Displacement     0.000482     0.001200     YES
 Predicted change in Energy=-1.143629D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.707141   -0.047053   -0.893740
      2          6           0        0.299602   -0.056236   -1.456984
      3          1           0        0.273605    0.001784   -2.548027
      4          6           0        1.747886   -0.103217    0.511973
      5          6           0       -0.326121   -1.407141   -0.963560
      6          1           0        0.219491   -2.238655   -1.420975
      7          6           0       -0.471756    1.068832   -0.792710
      8          6           0       -0.434930    1.027443    0.614071
      9          6           0        0.365068   -0.151877    1.182638
     10          6           0       -0.310236   -1.458030    0.578094
     11          1           0        0.232553   -2.327586    0.963856
     12          6           0       -1.176369    2.071512   -1.455427
     13          1           0       -1.207691    2.089183   -2.542431
     14          6           0       -1.109391    2.001224    1.350774
     15          1           0       -1.099767    1.979752    2.436379
     16          6           0       -1.809246    3.015483    0.684053
     17          1           0       -2.330980    3.775105    1.260243
     18          6           0       -1.844052    3.051733   -0.711351
     19          1           0       -2.392549    3.838502   -1.222400
     20          6           0        2.882313   -0.002797   -1.639179
     21          1           0        2.839239    0.040289   -2.725468
     22          6           0        4.118533   -0.006419   -0.979860
     23          1           0        5.039568    0.035640   -1.555311
     24          6           0        4.165356   -0.060901    0.414035
     25          1           0        5.124227   -0.061164    0.925895
     26          6           0        2.981251   -0.112758    1.163101
     27          1           0        3.036451   -0.153392    2.246821
     28          6           0       -1.791448   -1.540239   -1.341417
     29          6           0       -1.778101   -1.627784    0.954956
     30          8           0       -2.563590   -1.657956   -0.193185
     31          8           0       -2.272658   -1.746950    2.041062
     32          8           0       -2.285286   -1.558641   -2.433855
     33          6           0        0.421140   -0.202366    2.708977
     34          1           0        0.979286   -1.082225    3.047767
     35          1           0       -0.580433   -0.265794    3.140282
     36          1           0        0.917389    0.688840    3.108810
 ---------------------------------------------------------------------
                   Distance matrix (angstroms):
                   1          2          3          4          5
```

This journal is © The Royal Society of Chemistry 2014

1	C	0.000000				
2	C	1.516078	0.000000			
3	H	2.189537	1.092894	0.000000		
4	C	1.407425	2.444693	3.398254	0.000000	
5	C	2.447216	1.568420	2.203469	2.859882	0.000000
6	H	2.700777	2.184185	2.508533	3.260733	1.094685
7	C	2.450101	1.517245	2.185244	2.828905	2.486131
8	C	2.831343	2.450136	3.398950	2.460386	2.903095
9	C	2.474569	2.642165	3.734948	1.537642	2.580620
10	C	2.868268	2.545284	3.499223	2.464905	1.542576
11	H	3.290273	3.320239	4.214376	2.729148	2.207774
12	C	3.621938	2.589556	2.753174	4.141422	3.614676
13	H	3.972144	2.837772	2.559590	4.782409	3.936278
14	C	4.143203	3.755250	4.594680	3.646408	4.193639
15	H	4.803787	4.611047	5.535594	4.018859	4.860984
16	C	4.922757	4.297294	4.885385	4.733824	4.947110
17	H	5.962798	5.383536	5.960263	5.677890	5.985018
18	C	4.716642	3.848467	4.142468	4.934800	4.716915
19	H	5.658004	4.740431	4.856549	5.973977	5.643926
20	C	1.392361	2.589681	2.762496	2.434023	3.566889
21	H	2.155110	2.840445	2.572051	3.419455	3.901138
22	C	2.413272	3.848943	4.152432	2.802660	4.660176
23	H	3.398469	4.741877	4.868372	3.889488	5.587701
24	C	2.784474	4.294740	4.891163	2.419823	4.887075
25	H	3.871402	5.380998	5.966626	3.401878	5.923511
26	C	2.420386	3.749570	4.595317	1.394721	4.139665
27	H	3.411964	4.606295	5.536060	2.161623	4.815114
28	C	3.830162	2.566731	2.845731	4.245819	1.519104
29	C	4.250094	3.550220	4.374457	3.866927	2.416119
30	O	4.617892	3.515759	4.043475	4.637164	2.379633
31	O	5.228911	4.659545	5.531840	4.604861	3.596141
32	O	4.538317	3.145337	2.999314	5.202177	2.454190
33	C	3.828511	4.170295	5.263035	2.568445	3.936676
34	H	4.139666	4.669839	5.743341	2.824792	4.230887
35	H	4.642648	4.685427	5.758284	3.515040	4.267185
36	H	4.145558	4.667255	5.734658	2.839126	4.745909

		6	7	8	9	10
6	H	0.000000				
7	C	3.436861	0.000000			
8	C	3.903469	1.407871	0.000000		
9	C	3.339856	2.468280	1.534295	0.000000	
10	C	2.210490	2.879275	2.488859	1.589826	0.000000
11	H	2.386525	3.888088	3.438618	2.190692	1.095244
12	C	4.530689	1.393212	2.433646	3.778740	4.164500
13	H	4.693047	2.155050	3.418765	4.622993	4.808932
14	C	5.236897	2.422902	1.394947	2.614985	3.633473
15	H	5.866394	3.413383	2.160951	2.874275	3.986845
16	C	6.012727	2.785526	2.417839	3.874068	4.719172
17	H	7.061101	3.872369	3.400322	4.764021	5.651057
18	C	5.722760	2.412823	2.800022	4.327878	4.934899
19	H	6.617705	3.397815	3.886766	5.414036	5.969176
20	C	3.483862	3.621419	4.140366	3.784363	4.150467

This journal is © The Royal Society of Chemistry 2014

21	H	3.709227	3.969400	4.779872	4.629443	4.803923
22	C	4.514420	4.718256	4.933914	4.334288	4.914101
23	H	5.331379	5.658952	5.971602	5.420561	5.950032
24	C	4.866182	4.922940	4.731505	3.878301	4.691462
25	H	5.857107	5.962006	5.673317	4.766942	5.621885
26	C	4.338687	4.140604	3.643046	2.616548	3.603592
27	H	5.073097	4.800010	4.013817	2.875547	3.960687
28	C	2.130256	2.974882	3.501009	3.598467	2.425958
29	C	3.163635	3.468805	2.995085	2.612147	1.524949
30	O	3.096808	3.488635	3.520543	3.569062	2.390072
31	O	4.293982	4.382025	3.620884	3.199804	2.464721
32	O	2.786082	3.589689	4.404713	4.699190	3.603163
33	C	4.609083	3.830799	2.575639	1.528203	2.579199
34	H	4.678063	4.634849	3.517610	2.172905	2.811295
35	H	5.033600	4.154692	2.841721	2.176998	2.838880
36	H	5.438404	4.158842	2.857821	2.173016	3.538451

		11	12	13	14	15
11	H	0.000000				
12	C	5.214408	0.000000			
13	H	5.820326	1.087598	0.000000		
14	C	4.548528	2.807880	3.895439	0.000000	
15	H	4.743054	3.893641	4.981181	1.085860	0.000000
16	C	5.726746	2.422600	3.410293	1.401083	2.155630
17	H	6.625887	3.407378	4.308647	2.155720	2.474363
18	C	6.004638	1.400102	2.164327	2.428097	3.407537
19	H	7.049220	2.157696	2.491282	3.412229	4.302661
20	C	4.381970	4.561734	4.681921	5.374907	6.033046
21	H	5.100270	4.675892	4.539726	6.004389	6.776573
22	C	4.926122	5.707885	5.933114	6.065779	6.545702
23	H	5.919327	6.541607	6.649789	7.079446	7.576583
24	C	4.572429	6.047818	6.498707	5.740452	5.997972
25	H	5.391343	7.065161	7.533025	6.579662	6.721979
26	C	3.535604	5.377130	6.010553	4.608415	4.759679
27	H	3.772925	6.033630	6.780768	4.757444	4.657739
28	C	3.167141	3.665523	3.867287	4.500562	5.209655
29	C	2.128975	4.456098	5.135457	3.711272	3.958417
30	O	3.099284	4.174514	4.625848	4.229433	4.721261
31	O	2.788116	5.292252	6.071118	3.984783	3.926863
32	O	4.298282	3.919825	3.805210	5.327174	6.135541
33	C	2.756369	5.006478	5.956641	3.007167	2.673782
34	H	2.539925	5.905223	6.789036	4.092678	3.751261
35	H	3.106246	5.190249	6.183252	2.936241	2.409911
36	H	3.764126	5.208441	6.197858	2.986784	2.487476

		16	17	18	19	20
16	C	0.000000				
17	H	1.086843	0.000000			
18	C	1.396309	2.155818	0.000000		
19	H	2.156888	2.484215	1.086749	0.000000	
20	C	6.043025	7.060993	5.703468	6.538612	0.000000
21	H	6.487297	7.521030	5.921037	6.637562	1.087996
22	C	6.858503	7.804755	6.706476	7.565476	1.401055
23	H	7.797466	8.731319	7.562627	8.355175	2.159227

This journal is © The Royal Society of Chemistry 2014

24	C	6.725542	7.591666	6.860610	7.803165	2.421831
25	H	7.589287	8.390998	7.805614	8.736388	3.407226
26	C	5.741449	6.583670	6.067217	7.083840	2.806181
27	H	5.997065	6.724265	6.545450	7.579231	3.891971
28	C	4.985725	5.942442	4.635295	5.413533	4.929142
29	C	4.651267	5.439677	4.967777	5.915970	5.575803
30	O	4.814522	5.628918	4.792432	5.594604	5.872675
31	O	4.973630	5.577291	5.548589	6.470072	6.569625
32	O	5.556130	6.488243	4.941382	5.532475	5.454928
33	C	4.407890	5.049086	5.236307	6.300888	5.000367
34	H	5.491289	6.143839	6.260337	7.336017	5.172441
35	H	4.278998	4.788302	5.238111	6.257956	5.907879
36	H	4.327499	4.847075	5.272803	6.295668	5.184852

		21	22	23	24	25
21	H	0.000000				
22	C	2.164699	0.000000			
23	H	2.492135	1.086839	0.000000		
24	C	3.409590	1.395745	2.156824	0.000000	
25	H	4.308586	2.155532	2.484537	1.086938	0.000000
26	C	3.894169	2.428373	3.412983	1.402103	2.156681
27	H	4.979966	3.406460	4.301677	2.154550	2.472278
28	C	5.084971	6.116470	7.013696	6.383853	7.426637
29	C	6.135781	6.414252	7.453122	6.170284	7.077943
30	O	6.203793	6.928001	7.907697	6.942479	7.931242
31	O	7.214258	7.280298	8.341473	6.851131	7.668075
32	O	5.376093	6.747770	7.547653	7.208640	8.272318
33	C	5.953090	5.226531	6.290523	4.393851	5.031733
34	H	6.168444	5.218621	6.238897	4.258015	4.767121
35	H	6.796680	6.254848	7.329657	5.476944	6.122787
36	H	6.176805	5.239077	6.258838	4.286399	4.798448

		26	27	28	29	30
26	C	0.000000				
27	H	1.085886	0.000000			
28	C	5.575748	6.173120	0.000000		
29	C	4.999006	5.198332	2.298080	0.000000	
30	O	5.913747	6.291089	1.388704	1.391449	0.000000
31	O	5.571800	5.546927	3.422785	1.199339	2.254866
32	O	6.539501	7.225257	1.199014	3.427252	2.260070
33	C	2.991978	2.656282	4.805325	3.153581	4.410204
34	H	2.915424	2.395031	5.210728	3.504379	4.836032
35	H	4.076550	3.727298	4.814188	2.839908	4.121047
36	H	2.947519	2.437786	5.666667	4.155899	5.341145

		31	32	33	34	35
31	O	0.000000				
32	O	4.478895	0.000000			
33	C	3.176224	5.967659	0.000000		
34	H	3.468494	6.397857	1.095653	0.000000	
35	H	2.503145	5.970677	1.092335	1.762906	0.000000
36	H	4.153258	6.784499	1.095616	1.773197	1.776453

		36	
36	H	0.000000	

Stoichiometry C19H14O3

This journal is © The Royal Society of Chemistry 2014

```
 Framework group  C1[X(C19H14O3)]
 Deg. of freedom   102
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.707440   -0.053507   -0.893867
      2          6           0        0.299913   -0.047989   -1.457187
      3          1           0        0.274491    0.015251   -2.547953
      4          6           0        1.747604   -0.116459    0.511576
      5          6           0       -0.337452   -1.395702   -0.969977
      6          1           0        0.201011   -2.229779   -1.431181
      7          6           0       -0.461773    1.080625   -0.787787
      8          6           0       -0.425402    1.032475    0.618790
      9          6           0        0.364373   -0.156283    1.181971
     10          6           0       -0.322112   -1.453789    0.571429
     11          1           0        0.213143   -2.329744    0.953218
     12          6           0       -1.157681    2.092360   -1.445925
     13          1           0       -1.188776    2.115281   -2.532836
     14          6           0       -1.091503    2.008643    1.359927
     15          1           0       -1.082139    1.982116    2.445423
     16          6           0       -1.782552    3.031935    0.697840
     17          1           0       -2.297766    3.793374    1.277490
     18          6           0       -1.816950    3.074876   -0.697384
     19          1           0       -2.358616    3.868672   -1.204838
     20          6           0        2.883002   -0.015957   -1.639061
     21          1           0        2.840374    0.032475   -2.725142
     22          6           0        4.119099   -0.033245   -0.979729
     23          1           0        5.040502    0.003517   -1.554954
     24          6           0        4.165356   -0.094513    0.413903
     25          1           0        5.124154   -0.105378    0.925785
     26          6           0        2.980797   -0.139604    1.162689
     27          1           0        3.035570   -0.185676    2.246213
     28          6           0       -1.803846   -1.514444   -1.348482
     29          6           0       -1.791410   -1.612620    0.947466
     30          8           0       -2.577051   -1.630768   -0.200824
     31          8           0       -2.287049   -1.732498    2.033001
     32          8           0       -2.297749   -1.523588   -2.441007
     33          6           0        0.419904   -0.214244    2.708064
     34          1           0        0.970429   -1.100420    3.042835
     35          1           0       -0.582208   -0.271021    3.139045
     36          1           0        0.923780    0.670814    3.111990
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.4235734      0.2802086
0.2680763
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   446 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
```

```
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   446 basis functions,   760 primitive gaussians,   446 cartesian
basis functions
    76 alpha electrons       76 beta electrons
       nuclear repulsion energy      1805.8512067308 Hartrees.
 NAtoms=   36 NActive=   36 NUniq=   36 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   446 RedAO= T  NBF=   446
 NBsUse=   441 1.00D-06 NBFU=   441
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -958.192620185     A.U. after   11 cycles
            Convg  =    0.9760D-08             -V/T =  2.0094
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000019524    0.000024681    0.000011672
      2        6          -0.000009886   -0.000027191    0.000026436
      3        1           0.000009376    0.000007084   -0.000001528
      4        6           0.000014957   -0.000012553   -0.000033872
      5        6          -0.000004030    0.000157587   -0.000052311
      6        1          -0.000039393   -0.000004669   -0.000013334
      7        6           0.000006041    0.000002062    0.000011411
      8        6           0.000010349   -0.000003397    0.000003205
      9        6          -0.000047173    0.000003044    0.000031139
     10        6          -0.000049473   -0.000124689    0.000021895
     11        1           0.000028138    0.000006874   -0.000013862
     12        6          -0.000001264    0.000018864   -0.000001100
     13        1           0.000001296    0.000004450    0.000000584
     14        6           0.000004739    0.000007251    0.000006261
     15        1          -0.000003977   -0.000002048    0.000000448
     16        6           0.000004301    0.000000288    0.000007472
     17        1           0.000002766    0.000004076    0.000003694
     18        6           0.000001863   -0.000001054   -0.000004878
     19        1           0.000004202    0.000008286    0.000004953
     20        6          -0.000004727   -0.000000251   -0.000010010
     21        1           0.000003349   -0.000000012   -0.000000149
     22        6           0.000002455   -0.000007824    0.000004402
     23        1           0.000002503   -0.000002177    0.000001159
     24        6           0.000004136   -0.000002094   -0.000007385
     25        1           0.000001975   -0.000005680    0.000001536
     26        6          -0.000007663   -0.000010314    0.000010317
     27        1          -0.000002940   -0.000002586   -0.000000079
     28        6           0.000038192   -0.000458882    0.000088199
     29        6           0.000047665    0.000322997    0.000078919
     30        8          -0.000032483    0.000056680   -0.000092995
     31        8          -0.000000217   -0.000127540   -0.000040550
     32        8          -0.000018262    0.000172324   -0.000045086
     33        6           0.000012263    0.000011015   -0.000011987
     34        1          -0.000006498   -0.000004768    0.000006075
     35        1           0.000006775   -0.000002715    0.000004779
     36        1           0.000001124   -0.000007118    0.000004573
```

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000458882 RMS     0.000064855


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000083510 RMS     0.000019180
 Search for a local minimum.
 Step number   5 out of a maximum of  216
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
 DE=  1.16D-06 DEPred=-1.14D-06 R=-1.01D+00
 Trust test=-1.01D+00 RLast= 1.07D-02 DXMaxT set to 9.03D-02
     Eigenvalues ---    0.00402   0.00441   0.01073   0.01134
0.01161
     Eigenvalues ---    0.01420   0.01480   0.01560   0.01776
0.02002
     Eigenvalues ---    0.02111   0.02113   0.02128   0.02130
0.02131
     Eigenvalues ---    0.02134   0.02138   0.02147   0.02155
0.02156
     Eigenvalues ---    0.02159   0.02167   0.02741   0.03821
0.03985
     Eigenvalues ---    0.04567   0.04599   0.05169   0.05294
0.05431
     Eigenvalues ---    0.05506   0.05538   0.05607   0.05927
0.06450
     Eigenvalues ---    0.08287   0.08734   0.09415   0.10152
0.12697
     Eigenvalues ---    0.15813   0.15910   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16003
     Eigenvalues ---    0.16026   0.16390   0.20391   0.21665
0.22000
     Eigenvalues ---    0.22000   0.22356   0.22533   0.22626
0.24056
     Eigenvalues ---    0.24568   0.24592   0.24857   0.25172
0.26403
     Eigenvalues ---    0.27484   0.27583   0.28758   0.28918
0.29247
     Eigenvalues ---    0.29726   0.30099   0.34175   0.34222
0.34254
     Eigenvalues ---    0.34326   0.34484   0.34565   0.35082
0.35136
     Eigenvalues ---    0.35207   0.35216   0.35219   0.35229
0.35331
```

```
     Eigenvalues ---    0.35342   0.36607   0.39769   0.41769
0.42042
     Eigenvalues ---    0.42264   0.43361   0.44145   0.45247
0.45982
     Eigenvalues ---    0.46111   0.46186   0.46363   0.46611
0.46859
     Eigenvalues ---    1.03548
1.054201000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     5    4    3    2
1
 RFO step:  Lambda=-3.57959509D-07.
 DIIS coeffs:      0.38769      0.55348      0.01589      0.01095
0.03199
 Iteration  1 RMS(Cart)=  0.00044814 RMS(Int)=  0.00000062
 Iteration  2 RMS(Cart)=  0.00000030 RMS(Int)=  0.00000058
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86497   0.00001  -0.00007   0.00008   0.00000
2.86498
    R2        2.65965  -0.00001   0.00011  -0.00019  -0.00008
2.65957
    R3        2.63118   0.00001   0.00005  -0.00009  -0.00004
2.63114
    R4        2.06527   0.00000   0.00002  -0.00003  -0.00001
2.06526
    R5        2.96388   0.00001   0.00013  -0.00019  -0.00007
2.96382
    R6        2.86718   0.00002   0.00001   0.00004   0.00005
2.86722
    R7        2.90572   0.00002   0.00003   0.00000   0.00003
2.90575
    R8        2.63564   0.00000   0.00010  -0.00018  -0.00007
2.63557
    R9        2.06866  -0.00001  -0.00003   0.00003   0.00000
2.06866
   R10        2.91505   0.00003  -0.00006   0.00011   0.00005
2.91510
   R11        2.87069  -0.00002   0.00015  -0.00025  -0.00010
2.87058
   R12        2.66049   0.00000   0.00007  -0.00010  -0.00003
2.66046
   R13        2.63279   0.00002   0.00003  -0.00004  -0.00001
2.63278
   R14        2.89940   0.00000   0.00009  -0.00016  -0.00007
2.89933
   R15        2.63607   0.00001   0.00003  -0.00006  -0.00002
2.63605
   R16        3.00433   0.00001   0.00003   0.00003   0.00006
3.00439
```

This journal is © The Royal Society of Chemistry 2014

R17	2.88789	0.00001	0.00009	-0.00012	-0.00003
2.88786					
R18	2.06971	0.00001	0.00001	-0.00001	0.00000
2.06971					
R19	2.88174	-0.00003	0.00020	-0.00030	-0.00009
2.88164					
R20	2.05526	0.00000	0.00002	-0.00003	-0.00001
2.05525					
R21	2.64581	0.00000	0.00006	-0.00011	-0.00005
2.64576					
R22	2.05198	0.00000	0.00001	-0.00002	-0.00001
2.05197					
R23	2.64766	0.00000	0.00006	-0.00011	-0.00005
2.64762					
R24	2.05384	0.00000	0.00002	-0.00002	-0.00001
2.05383					
R25	2.63864	0.00000	0.00004	-0.00008	-0.00004
2.63860					
R26	2.05366	0.00000	0.00002	-0.00002	-0.00001
2.05365					
R27	2.05601	0.00000	0.00002	-0.00004	-0.00001
2.05600					
R28	2.64761	0.00001	0.00005	-0.00009	-0.00004
2.64757					
R29	2.05383	0.00000	0.00002	-0.00003	-0.00001
2.05382					
R30	2.63758	0.00000	0.00004	-0.00007	-0.00004
2.63754					
R31	2.05401	0.00000	0.00002	-0.00002	-0.00001
2.05401					
R32	2.64959	0.00001	0.00004	-0.00007	-0.00003
2.64956					
R33	2.05203	0.00000	-0.00001	0.00001	0.00000
2.05203					
R34	2.62427	-0.00005	0.00009	-0.00019	-0.00010
2.62417					
R35	2.26581	0.00004	-0.00006	0.00007	0.00002
2.26582					
R36	2.62946	0.00007	-0.00013	0.00023	0.00010
2.62956					
R37	2.26642	-0.00002	0.00002	-0.00005	-0.00003
2.26639					
R38	2.07048	0.00000	0.00001	-0.00002	-0.00001
2.07047					
R39	2.06421	-0.00001	0.00000	-0.00002	-0.00002
2.06419					
R40	2.07041	0.00000	-0.00001	0.00001	0.00000
2.07042					
A1	1.97980	0.00000	-0.00001	-0.00004	-0.00005
1.97975					
A2	2.19553	0.00000	0.00002	0.00000	0.00002
2.19555					

This journal is © The Royal Society of Chemistry 2014

A3	2.10780	0.00000	-0.00001	0.00003	0.00003
2.10782					
A4	1.97430	-0.00001	0.00006	-0.00014	-0.00008
1.97422					
A5	1.83250	0.00001	-0.00003	-0.00008	-0.00011
1.83239					
A6	1.88058	-0.00001	0.00003	-0.00006	-0.00004
1.88054					
A7	1.92869	-0.00001	-0.00001	0.00002	0.00001
1.92870					
A8	1.96667	0.00000	-0.00003	0.00006	0.00003
1.96670					
A9	1.87352	0.00001	-0.00001	0.00021	0.00019
1.87371					
A10	1.99420	0.00001	0.00002	0.00002	0.00004
1.99424					
A11	2.08536	0.00000	-0.00006	0.00007	0.00002
2.08538					
A12	2.20363	-0.00001	0.00004	-0.00010	-0.00006
2.20357					
A13	1.90070	0.00001	-0.00008	0.00013	0.00005
1.90074					
A14	1.91635	-0.00002	0.00004	-0.00006	-0.00002
1.91633					
A15	1.96280	0.00004	0.00007	0.00008	0.00015
1.96295					
A16	1.96862	0.00002	0.00006	-0.00008	-0.00002
1.96860					
A17	1.88629	-0.00004	-0.00011	-0.00007	-0.00018
1.88611					
A18	1.82930	0.00000	0.00003	0.00000	0.00002
1.82932					
A19	1.98491	0.00000	0.00000	0.00002	0.00002
1.98493					
A20	2.19263	0.00000	0.00000	0.00000	0.00000
2.19263					
A21	2.10563	0.00000	0.00000	-0.00002	-0.00002
2.10561					
A22	1.98944	0.00000	0.00001	-0.00004	-0.00004
1.98940					
A23	2.08811	0.00000	-0.00002	0.00004	0.00002
2.08813					
A24	2.20553	0.00001	0.00001	0.00000	0.00001
2.20555					
A25	1.85767	0.00000	0.00004	-0.00009	-0.00005
1.85763					
A26	1.81537	-0.00001	0.00007	0.00008	0.00014
1.81551					
A27	1.98633	0.00000	0.00013	-0.00028	-0.00016
1.98618					
A28	1.84326	0.00000	-0.00016	0.00009	-0.00007
1.84318					

This journal is © The Royal Society of Chemistry 2014

A29	1.99835	0.00000	0.00001	-0.00002	-0.00001
1.99834					
A30	1.94791	0.00002	-0.00009	0.00024	0.00015
1.94805					
A31	1.93617	0.00001	0.00000	-0.00004	-0.00004
1.93613					
A32	1.96416	-0.00001	-0.00006	0.00007	0.00001
1.96417					
A33	1.81393	0.00000	0.00002	-0.00008	-0.00006
1.81387					
A34	1.88371	-0.00001	0.00016	-0.00019	-0.00003
1.88368					
A35	1.98925	-0.00002	-0.00017	0.00004	-0.00013
1.98912					
A36	1.87718	0.00003	0.00004	0.00022	0.00026
1.87744					
A37	2.09633	0.00000	-0.00002	0.00002	0.00000
2.09633					
A38	2.08546	0.00000	0.00001	-0.00001	0.00000
2.08546					
A39	2.10139	0.00000	0.00000	0.00000	0.00000
2.10139					
A40	2.10588	0.00000	-0.00006	0.00009	0.00003
2.10591					
A41	2.08926	0.00000	0.00002	-0.00004	-0.00002
2.08924					
A42	2.08804	0.00000	0.00004	-0.00005	-0.00001
2.08803					
A43	2.08687	0.00000	0.00001	-0.00001	0.00000
2.08687					
A44	2.10226	0.00000	-0.00001	0.00002	0.00001
2.10227					
A45	2.09404	0.00000	0.00000	-0.00001	-0.00001
2.09404					
A46	2.09559	0.00000	-0.00001	0.00002	0.00001
2.09560					
A47	2.09166	0.00000	-0.00001	0.00002	0.00001
2.09167					
A48	2.09593	0.00000	0.00002	-0.00004	-0.00002
2.09591					
A49	2.09715	0.00000	-0.00004	0.00007	0.00003
2.09718					
A50	2.08598	0.00000	0.00003	-0.00007	-0.00003
2.08594					
A51	2.10004	0.00000	0.00000	0.00000	0.00000
2.10005					
A52	2.09264	0.00000	0.00000	-0.00001	0.00000
2.09264					
A53	2.09401	0.00000	0.00000	0.00001	0.00000
2.09401					
A54	2.09653	0.00000	0.00000	0.00000	0.00000
2.09653					

```
   A55        2.09428   0.00000  -0.00001   0.00001   0.00000
2.09428
   A56        2.10209   0.00000  -0.00001   0.00003   0.00001
2.10210
   A57        2.08682   0.00000   0.00003  -0.00004  -0.00001
2.08680
   A58        2.09111   0.00000   0.00005  -0.00007  -0.00003
2.09108
   A59        2.10729   0.00000  -0.00001  -0.00001  -0.00002
2.10727
   A60        2.08476   0.00000  -0.00004   0.00008   0.00005
2.08481
   A61        1.91569   0.00002  -0.00010   0.00016   0.00006
1.91575
   A62        2.24626  -0.00003   0.00007  -0.00016  -0.00008
2.24618
   A63        2.12121   0.00001   0.00004   0.00000   0.00004
2.12125
   A64        1.91971   0.00000  -0.00007   0.00012   0.00005
1.91976
   A65        2.25464   0.00003  -0.00003   0.00004   0.00001
2.25466
   A66        2.10866  -0.00002   0.00004  -0.00016  -0.00011
2.10855
   A67        1.94609  -0.00001   0.00013  -0.00020  -0.00007
1.94601
   A68        1.93270   0.00001  -0.00008   0.00013   0.00005
1.93275
   A69        1.94190   0.00001   0.00004  -0.00007  -0.00002
1.94187
   A70        1.93290   0.00000  -0.00008   0.00014   0.00006
1.93296
   A71        1.87378  -0.00001   0.00008  -0.00013  -0.00005
1.87373
   A72        1.88561  -0.00001  -0.00001  -0.00002  -0.00003
1.88558
   A73        1.89488  -0.00001   0.00005  -0.00006  -0.00001
1.89488
    D1        3.12738   0.00000   0.00018  -0.00006   0.00012
3.12750
    D2       -1.05137  -0.00001   0.00018  -0.00017   0.00001  -
1.05136
    D3        0.94166   0.00000   0.00016   0.00000   0.00016
0.94182
    D4       -0.02552  -0.00001   0.00014  -0.00029  -0.00015  -
0.02567
    D5        2.07892  -0.00001   0.00014  -0.00040  -0.00026
2.07866
    D6       -2.21125   0.00000   0.00012  -0.00023  -0.00011  -
2.21135
    D7       -0.00718  -0.00001  -0.00026   0.00000  -0.00025  -
0.00743
```

This journal is © The Royal Society of Chemistry 2014

D8	3.13239	0.00000	-0.00009	0.00000	-0.00009	3.13230
D9	-3.13810	-0.00001	-0.00022	0.00022	0.00000	-3.13810
D10	0.00147	0.00000	-0.00006	0.00022	0.00016	0.00163
D11	0.01189	0.00000	0.00010	0.00003	0.00013	0.01202
D12	-3.13607	0.00000	0.00005	0.00015	0.00020	-3.13587
D13	3.14141	0.00000	0.00006	-0.00021	-0.00015	3.14126
D14	-0.00656	0.00000	0.00001	-0.00010	-0.00009	-0.00664
D15	-1.13386	-0.00001	0.00023	0.00043	0.00066	-1.13320
D16	1.02949	0.00000	0.00028	0.00038	0.00065	1.03015
D17	3.05903	0.00001	0.00038	0.00038	0.00076	3.05979
D18	1.00045	-0.00001	0.00028	0.00022	0.00050	1.00095
D19	-3.11938	0.00000	0.00033	0.00017	0.00050	-3.11888
D20	-1.08985	0.00001	0.00043	0.00017	0.00060	-1.08924
D21	-3.13182	-0.00001	0.00022	0.00044	0.00067	-3.13115
D22	-0.96846	0.00000	0.00027	0.00039	0.00066	-0.96780
D23	1.06107	0.00001	0.00037	0.00040	0.00077	1.06184
D24	-0.93465	-0.00001	0.00002	0.00010	0.00012	-0.93453
D25	2.21404	-0.00001	0.00013	-0.00021	-0.00008	2.21396
D26	-3.12491	0.00001	-0.00005	0.00028	0.00023	-3.12469
D27	0.02378	0.00000	0.00006	-0.00003	0.00003	0.02381
D28	1.03090	0.00001	-0.00001	0.00008	0.00007	1.03096
D29	-2.10360	0.00001	0.00010	-0.00023	-0.00013	-2.10373
D30	-0.91656	0.00000	0.00023	-0.00016	0.00007	-0.91648
D31	1.02551	0.00000	0.00010	-0.00006	0.00004	1.02554
D32	-3.13423	0.00001	0.00010	0.00013	0.00022	-3.13400
D33	2.22722	0.00000	0.00006	-0.00016	-0.00010	2.22712

This journal is © The Royal Society of Chemistry 2014

D34	-2.11390	-0.00001	-0.00008	-0.00006	-0.00014	-2.11404
D35	0.00956	0.00000	-0.00008	0.00013	0.00005	0.00960
D36	0.00458	0.00000	0.00008	-0.00021	-0.00013	0.00444
D37	3.13909	0.00000	-0.00003	-0.00013	-0.00016	3.13893
D38	-3.13931	0.00001	0.00026	-0.00021	0.00005	-3.13926
D39	-0.00480	0.00000	0.00016	-0.00013	0.00003	-0.00477
D40	-0.02575	0.00000	-0.00044	-0.00045	-0.00089	-0.02663
D41	-2.13825	0.00001	-0.00060	-0.00023	-0.00083	-2.13908
D42	2.11922	-0.00002	-0.00063	-0.00047	-0.00110	2.11812
D43	2.09747	0.00001	-0.00048	-0.00038	-0.00085	2.09661
D44	-0.01504	0.00002	-0.00064	-0.00016	-0.00079	-0.01583
D45	-2.04075	-0.00002	-0.00067	-0.00040	-0.00107	-2.04182
D46	-2.13777	-0.00004	-0.00056	-0.00050	-0.00107	-2.13884
D47	2.03291	-0.00003	-0.00072	-0.00028	-0.00101	2.03190
D48	0.00720	-0.00006	-0.00076	-0.00052	-0.00128	0.00592
D49	-2.08239	0.00007	0.00046	0.00094	0.00140	-2.08099
D50	1.06731	-0.00007	-0.00254	0.00046	-0.00207	1.06524
D51	2.10215	0.00006	0.00059	0.00078	0.00137	2.10353
D52	-1.03133	-0.00008	-0.00240	0.00030	-0.00210	-1.03343
D53	-0.00131	0.00006	0.00057	0.00091	0.00147	0.00016
D54	-3.13480	-0.00007	-0.00243	0.00043	-0.00200	-3.13680
D55	-0.00941	0.00000	-0.00007	-0.00022	-0.00030	-0.00971
D56	-3.13631	0.00000	0.00006	-0.00018	-0.00012	-3.13642
D57	3.12548	0.00000	-0.00018	0.00007	-0.00011	3.12537
D58	-0.00142	0.00000	-0.00004	0.00011	0.00007	-0.00135
D59	0.00366	0.00000	-0.00021	0.00041	0.00020	0.00386

This journal is © The Royal Society of Chemistry 2014

D60	-3.14017	0.00000	-0.00006	0.00018	0.00012	-3.14005
D61	-3.13038	0.00000	-0.00009	0.00008	-0.00001	-3.13039
D62	0.00897	0.00000	0.00006	-0.00015	-0.00009	0.00888
D63	0.92375	0.00000	-0.00005	0.00025	0.00020	0.92396
D64	-0.99881	0.00001	-0.00007	0.00016	0.00009	-0.99872
D65	3.13423	-0.00001	0.00016	-0.00020	-0.00004	3.13419
D66	-2.23370	0.00000	-0.00020	0.00021	0.00001	-2.23369
D67	2.12692	0.00001	-0.00022	0.00012	-0.00010	2.12682
D68	-0.02322	-0.00001	0.00001	-0.00024	-0.00023	-0.02345
D69	3.13149	0.00000	0.00012	-0.00030	-0.00018	3.13131
D70	-0.00727	0.00000	0.00000	-0.00001	-0.00002	-0.00728
D71	0.00657	0.00000	0.00027	-0.00025	0.00002	0.00660
D72	-3.13218	0.00000	0.00015	0.00004	0.00019	-3.13200
D73	-0.96741	0.00000	0.00034	0.00031	0.00065	-0.96676
D74	1.19188	-0.00001	0.00037	0.00025	0.00062	1.19250
D75	-3.00747	0.00001	0.00042	0.00041	0.00084	-3.00663
D76	0.98512	0.00000	0.00035	0.00028	0.00063	0.98576
D77	-3.13877	-0.00001	0.00038	0.00021	0.00060	-3.13817
D78	-1.05493	0.00001	0.00044	0.00038	0.00082	-1.05411
D79	-3.11621	0.00001	0.00020	0.00047	0.00067	-3.11554
D80	-0.95692	-0.00001	0.00023	0.00040	0.00063	-0.95629
D81	1.12692	0.00002	0.00028	0.00057	0.00085	1.12777
D82	-1.02963	0.00000	0.00054	-0.00100	-0.00046	-1.03009
D83	-3.11212	0.00000	0.00046	-0.00087	-0.00041	-3.11253
D84	1.06183	0.00000	0.00042	-0.00085	-0.00043	1.06140
D85	3.11123	0.00000	0.00036	-0.00063	-0.00026	3.11097

This journal is © The Royal Society of Chemistry 2014

D86	1.02874	0.00001	0.00029	-0.00050	-0.00022	1.02852
D87	-1.08050	0.00000	0.00025	-0.00048	-0.00023	-1.08073
D88	1.01851	-0.00001	0.00064	-0.00092	-0.00028	1.01824
D89	-1.06397	-0.00001	0.00056	-0.00079	-0.00023	-1.06421
D90	3.10997	-0.00001	0.00052	-0.00077	-0.00025	3.10972
D91	-0.01111	0.00004	0.00074	0.00000	0.00074	-0.01037
D92	3.11031	-0.00005	-0.00136	-0.00023	-0.00159	3.10872
D93	2.09859	0.00004	0.00066	-0.00008	0.00058	2.09917
D94	-1.06317	-0.00005	-0.00144	-0.00031	-0.00175	-1.06492
D95	-2.09707	0.00004	0.00078	-0.00014	0.00064	-2.09643
D96	1.02436	-0.00005	-0.00132	-0.00037	-0.00169	1.02267
D97	-0.00782	0.00000	-0.00003	0.00009	0.00006	-0.00777
D98	3.13788	0.00000	0.00001	-0.00001	0.00000	3.13789
D99	3.13152	0.00000	0.00012	-0.00014	-0.00002	3.13150
D100	-0.00596	0.00000	0.00016	-0.00024	-0.00008	-0.00604
D101	-3.13777	0.00000	0.00000	-0.00001	-0.00001	-3.13778
D102	0.00842	0.00000	0.00003	-0.00005	-0.00002	0.00840
D103	0.00663	0.00000	-0.00012	0.00027	0.00015	0.00678
D104	-3.13037	0.00000	-0.00009	0.00023	0.00014	-3.13022
D105	-0.00084	0.00000	-0.00001	0.00001	-0.00001	-0.00084
D106	3.13663	0.00000	-0.00006	0.00011	0.00005	3.13668
D107	-3.13782	0.00000	0.00002	-0.00003	-0.00001	-3.13783
D108	-0.00035	0.00000	-0.00002	0.00007	0.00005	-0.00030
D109	-3.13345	0.00000	-0.00005	0.00010	0.00005	-3.13340
D110	0.00559	0.00000	0.00002	-0.00003	-0.00001	0.00557
D111	0.00176	0.00000	-0.00010	0.00022	0.00012	0.00188

```
   D112        3.14080   0.00000  -0.00003   0.00008   0.00005
3.14085
   D113       -3.13887   0.00000   0.00001   0.00005   0.00006  -
3.13881
   D114        0.00043   0.00000   0.00000   0.00004   0.00004
0.00047
   D115        0.00016   0.00000   0.00007  -0.00008  -0.00001
0.00015
   D116        3.13946   0.00000   0.00007  -0.00010  -0.00003
3.13943
   D117       -0.00554   0.00000  -0.00005   0.00009   0.00004  -
0.00551
   D118       -3.14014   0.00000   0.00005   0.00001   0.00006  -
3.14008
   D119        3.13377   0.00000  -0.00005   0.00007   0.00002
3.13379
   D120       -0.00083   0.00000   0.00005  -0.00001   0.00004  -
0.00079
   D121       -0.00598  -0.00004  -0.00011  -0.00096  -0.00107  -
0.00704
   D122        3.12819   0.00008   0.00263  -0.00052   0.00212
3.13031
   D123        0.01098   0.00000  -0.00042   0.00060   0.00018
0.01116
   D124       -3.11241   0.00008   0.00148   0.00081   0.00228  -
3.11013
         Item               Value     Threshold  Converged?
 Maximum Force            0.000084     0.000450     YES
 RMS     Force            0.000019     0.000300     YES
 Maximum Displacement     0.002437     0.001800     NO
 RMS     Displacement     0.000448     0.001200     YES
 Predicted change in Energy=-8.752822D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.707057   -0.046972   -0.893730
      2          6           0        0.299472   -0.056339   -1.456861
      3          1           0        0.273468    0.001675   -2.547899
      4          6           0        1.747852   -0.103276    0.511935
      5          6           0       -0.325821   -1.407405   -0.963446
      6          1           0        0.220349   -2.238790   -1.420428
      7          6           0       -0.471928    1.068704   -0.792536
      8          6           0       -0.434844    1.027475    0.614225
      9          6           0        0.365070   -0.151892    1.182716
     10          6           0       -0.310567   -1.457948    0.578254
     11          1           0        0.231754   -2.327605    0.964439
```

This journal is © The Royal Society of Chemistry 2014

12	6	0	-1.176618	2.071345	-1.455214
13	1	0	-1.208145	2.088916	-2.542206
14	6	0	-1.109177	2.001305	1.350956
15	1	0	-1.099498	1.979872	2.436555
16	6	0	-1.809148	3.015468	0.684264
17	1	0	-2.330801	3.775132	1.260463
18	6	0	-1.844187	3.051591	-0.711118
19	1	0	-2.392748	3.838336	-1.222126
20	6	0	2.882167	-0.002737	-1.639230
21	1	0	2.839061	0.040317	-2.725510
22	6	0	4.118386	-0.006419	-0.979957
23	1	0	5.039401	0.035671	-1.555431
24	6	0	4.165252	-0.060920	0.413916
25	1	0	5.124135	-0.061176	0.925744
26	6	0	2.981194	-0.112786	1.163024
27	1	0	3.036391	-0.153381	2.246747
28	6	0	-1.790837	-1.541528	-1.341924
29	6	0	-1.778659	-1.626679	0.954490
30	8	0	-2.563650	-1.657583	-0.194038
31	8	0	-2.273636	-1.746754	2.040284
32	8	0	-2.284266	-1.558615	-2.434578
33	6	0	0.421494	-0.202216	2.709032
34	1	0	0.979330	-1.082258	3.047841
35	1	0	-0.579998	-0.265202	3.140560
36	1	0	0.918191	0.688816	3.108696

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.516080	0.000000			
3	H	2.189479	1.092888	0.000000		
4	C	1.407384	2.444620	3.398148	0.000000	
5	C	2.447086	1.568384	2.203439	2.859654	0.000000
6	H	2.700328	2.184188	2.508724	3.260017	1.094685
7	C	2.450091	1.517270	2.185283	2.828888	2.486296
8	C	2.831273	2.450158	3.398970	2.460330	2.903372
9	C	2.474584	2.642121	3.734898	1.537659	2.580630
10	C	2.868518	2.545260	3.499204	2.465081	1.542604
11	H	3.290988	3.320532	4.214713	2.729644	2.207804
12	C	3.621894	2.589573	2.753224	4.141398	3.614885
13	H	3.972139	2.837781	2.559645	4.782405	3.936399
14	C	4.143095	3.755268	4.594704	3.646346	4.193973
15	H	4.803712	4.611071	5.535620	4.018840	4.861299
16	C	4.922631	4.297289	4.885398	4.733763	4.947424
17	H	5.962661	5.383527	5.960270	5.677830	5.985349
18	C	4.716543	3.848460	4.142489	4.934754	4.717176
19	H	5.657903	4.740427	4.856578	5.973930	5.644191
20	C	1.392340	2.589680	2.762428	2.433986	3.566646
21	H	2.155103	2.840479	2.572024	3.419416	3.900929
22	C	2.413212	3.848901	4.152337	2.802598	4.659829
23	H	3.398411	4.741846	4.868292	3.889422	5.587353
24	C	2.784395	4.294658	4.891038	2.419758	4.886705

This journal is © The Royal Society of Chemistry 2014

25	H	3.871319	5.380911	5.966499	3.401808	5.923123
26	C	2.420329	3.749482	4.595196	1.394683	4.139355
27	H	3.411898	4.606176	5.535920	2.161577	4.814809
28	C	3.830122	2.566786	2.845559	4.245902	1.519048
29	C	4.249894	3.549536	4.373727	3.866896	2.416049
30	O	4.617637	3.515135	4.042652	4.637167	2.379592
31	O	5.229112	4.659229	5.531380	4.605348	3.596044
32	O	4.537613	3.144592	2.998224	5.201723	2.454099
33	C	3.828403	4.170233	5.262966	2.568316	3.936757
34	H	4.139732	4.669803	5.743296	2.824863	4.230787
35	H	4.642601	4.685443	5.758315	3.514936	4.267564
36	H	4.145251	4.667160	5.734535	2.838822	4.745950

		6	7	8	9	10
6	H	0.000000				
7	C	3.437006	0.000000			
8	C	3.903534	1.407854	0.000000		
9	C	3.339528	2.468206	1.534260	0.000000	
10	C	2.210502	2.879075	2.488789	1.589856	0.000000
11	H	2.386548	3.888065	3.438542	2.190695	1.095241
12	C	4.531004	1.393205	2.433612	3.778659	4.164247
13	H	4.693401	2.155039	3.418728	4.622907	4.808655
14	C	5.237043	2.422890	1.394935	2.614951	3.633357
15	H	5.866467	3.413372	2.160952	2.874282	3.986766
16	C	6.012970	2.785496	2.417795	3.873997	4.718944
17	H	7.061360	3.872334	3.400279	4.763957	5.650831
18	C	5.723073	2.412793	2.799969	4.327786	4.934614
19	H	6.618086	3.397787	3.886709	5.413940	5.968875
20	C	3.483257	3.621440	4.140285	3.784363	4.150714
21	H	3.708803	3.969460	4.779829	4.629450	4.804145
22	C	4.513556	4.718263	4.933788	4.334247	4.914324
23	H	5.330540	5.658967	5.971469	5.420516	5.950266
24	C	4.865202	4.922907	4.731344	3.878236	4.691658
25	H	5.856077	5.961966	5.673134	4.766861	5.622073
26	C	4.337785	4.140554	3.642896	2.616490	3.603763
27	H	5.072198	4.799900	4.013605	2.875434	3.960794
28	C	2.130072	2.975678	3.502144	3.599004	2.425957
29	C	3.164008	3.467669	2.994353	2.612021	1.524899
30	O	3.097174	3.488000	3.520603	3.569308	2.390120
31	O	4.294018	4.381533	3.620932	3.200278	2.464666
32	O	2.786438	3.589383	4.404931	4.699219	3.603162
33	C	4.608745	3.830721	2.575592	1.528187	2.579339
34	H	4.677504	4.634790	3.517577	2.172921	2.811376
35	H	5.033709	4.154544	2.841559	2.176958	2.839128
36	H	5.437906	4.158889	2.857933	2.173046	3.538584

		11	12	13	14	15
11	H	0.000000				
12	C	5.214307	0.000000			
13	H	5.820269	1.087591	0.000000		
14	C	4.548292	2.807854	3.895405	0.000000	
15	H	4.742755	3.893608	4.981140	1.085854	0.000000
16	C	5.726448	2.422566	3.410251	1.401058	2.155594
17	H	6.625536	3.407335	4.308593	2.155694	2.474320

This journal is © The Royal Society of Chemistry 2014

18	C	6.004397	1.400075	2.164296	2.428063	3.407490
19	H	7.048965	2.157674	2.491258	3.412182	4.302596
20	C	4.382784	4.561734	4.681990	5.374777	6.032945
21	H	5.101062	4.675939	4.539849	6.004302	6.776507
22	C	4.926915	5.707893	5.933210	6.065603	6.545551
23	H	5.920160	6.541629	6.649915	7.079253	7.576408
24	C	4.573112	6.047791	6.498757	5.740246	5.997792
25	H	5.391994	7.065132	7.533083	6.579424	6.721759
26	C	3.536139	5.377081	6.010555	4.608236	4.759533
27	H	3.773269	6.033520	6.780712	4.757190	4.657508
28	C	3.166718	3.666464	3.867859	4.501992	5.211057
29	C	2.129121	4.454717	5.134005	3.710479	3.957902
30	O	3.099239	4.173647	4.624667	4.229653	4.721742
31	O	2.787796	5.291488	6.070161	3.984857	3.927260
32	O	4.298257	3.919521	3.804484	5.327676	6.136163
33	C	2.756245	5.006395	5.956552	3.007130	2.673794
34	H	2.539749	5.905152	6.788962	4.092632	3.751245
35	H	3.106115	5.190044	6.183064	2.935945	2.409536
36	H	3.764018	5.208540	6.197925	2.987056	2.487905

		16	17	18	19	20
16	C	0.000000				
17	H	1.086838	0.000000			
18	C	1.396289	2.155791	0.000000		
19	H	2.156855	2.484166	1.086745	0.000000	
20	C	6.042898	7.060846	5.703397	6.538543	0.000000
21	H	6.487212	7.520924	5.921010	6.637540	1.087988
22	C	6.858360	7.804591	6.706414	7.565425	1.401033
23	H	7.797310	8.731134	7.562568	8.355130	2.159202
24	C	6.725378	7.591486	6.860524	7.803089	2.421797
25	H	7.589102	8.390791	7.805521	8.736307	3.407187
26	C	5.741303	6.583517	6.067124	7.083753	2.806161
27	H	5.996850	6.724041	6.545293	7.579079	3.891952
28	C	4.987182	5.943977	4.636541	5.414756	4.928817
29	C	4.650105	5.438570	4.966362	5.914486	5.575649
30	O	4.814363	5.628871	4.791798	5.593863	5.872310
31	O	4.973258	5.576973	5.547861	6.469215	6.569834
32	O	5.556540	6.488786	4.941456	5.532529	5.453931
33	C	4.407828	5.049038	5.236220	6.300796	5.000208
34	H	5.491216	6.143771	6.260250	7.335923	5.172503
35	H	4.278668	4.787942	5.237817	6.257645	5.907780
36	H	4.327766	4.847398	5.272990	6.295857	5.184423

		21	22	23	24	25
21	H	0.000000				
22	C	2.164674	0.000000			
23	H	2.492109	1.086835	0.000000		
24	C	3.409550	1.395725	2.156801	0.000000	
25	H	4.308541	2.155510	2.484509	1.086933	0.000000
26	C	3.894142	2.428351	3.412953	1.402087	2.156655
27	H	4.979940	3.406454	4.301667	2.154564	2.472291
28	C	5.084535	6.116085	7.013222	6.383586	7.426345
29	C	6.135520	6.414239	7.453123	6.170405	7.078148
30	O	6.203265	6.927743	7.907394	6.942411	7.931234

31	O	7.214297	7.280698	8.341865	6.851744	7.668793
32	O	5.374914	6.746791	7.546571	7.207863	8.271547
33	C	5.952957	5.226279	6.290254	4.393546	5.031385
34	H	6.168497	5.218645	6.238914	4.258027	4.767108
35	H	6.796623	6.254634	7.329427	5.476652	6.122432
36	H	6.176427	5.238481	6.258198	4.285715	4.797680

		26	27	28	29	30
26	C	0.000000				
27	H	1.085887	0.000000			
28	C	5.575692	6.173139	0.000000		
29	C	4.999155	5.198581	2.298024	0.000000	
30	O	5.913824	6.291305	1.388651	1.391504	0.000000
31	O	5.572492	5.547779	3.422652	1.199321	2.254830
32	O	6.538977	7.224879	1.199023	3.427251	2.260059
33	C	2.991689	2.655895	4.806081	3.154074	4.411009
34	H	2.915454	2.395009	5.211026	3.504998	4.836681
35	H	4.076269	3.726885	4.815372	2.840653	4.122275
36	H	2.946894	2.437011	5.667564	4.156335	5.341990

		31	32	33	34	35
31	O	0.000000				
32	O	4.478828	0.000000			
33	C	3.177506	5.968055	0.000000		
34	H	3.469655	6.398037	1.095648	0.000000	
35	H	2.504798	5.971567	1.092323	1.762861	0.000000
36	H	4.154667	6.784877	1.095617	1.773173	1.776439

		36
36	H	0.000000

Stoichiometry C19H14O3
Framework group C1[X(C19H14O3)]
Deg. of freedom 102
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.707351	-0.055712	-0.893665
2	6	0	0.299761	-0.051863	-1.456847
3	1	0	0.274301	0.008548	-2.547767
4	6	0	1.747603	-0.115166	0.511887
5	6	0	-0.337137	-1.398487	-0.966141
6	1	0	0.201889	-2.233621	-1.424767
7	6	0	-0.461973	1.078439	-0.790299
8	6	0	-0.425302	1.034090	0.616378
9	6	0	0.364427	-0.153238	1.182536
10	6	0	-0.322381	-1.452233	0.575455
11	1	0	0.212432	-2.327286	0.959918
12	6	0	-1.157996	2.088418	-1.450993
13	1	0	-1.189325	2.108425	-2.537949
14	6	0	-1.091275	2.012206	1.355034

```
     15          1           0       -1.081825    1.988527    2.440588
     16          6           0       -1.782479    3.033672    0.690348
     17          1           0       -2.297611    3.796640    1.268047
     18          6           0       -1.817149    3.072877   -0.704960
     19          1           0       -2.358910    3.865323   -1.214412
     20          6           0        2.882828   -0.020088   -1.639046
     21          1           0        2.840138    0.025501   -2.725240
     22          6           0        4.118943   -0.035705   -0.979752
     23          1           0        5.040309   -0.000382   -1.555118
     24          6           0        4.165282   -0.093385    0.414010
     25          1           0        5.124106   -0.102899    0.925860
     26          6           0        2.980790   -0.136570    1.162985
     27          1           0        3.035592   -0.179798    2.246626
     28          6           0       -1.803235   -1.519265   -1.344922
     29          6           0       -1.791884   -1.609094    0.951318
     30          8           0       -2.577065   -1.630964   -0.197288
     31          8           0       -2.287919   -1.727077    2.036859
     32          8           0       -2.296748   -1.529933   -2.437619
     33          6           0        0.420353   -0.207087    2.708750
     34          1           0        0.970593   -1.092563    3.045817
     35          1           0       -0.581661   -0.262327    3.140128
     36          1           0        0.924670    0.678846    3.110202
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.4235828      0.2802140
0.2680871
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   446 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   446 basis functions,   760 primitive gaussians,   446 cartesian
basis functions
    76 alpha electrons       76 beta electrons
       nuclear repulsion energy      1805.8683069059 Hartrees.
 NAtoms=   36 NActive=   36 NUniq=   36 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   446 RedAO= T  NBF=   446
 NBsUse=   441 1.00D-06 NBFU=   441
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -958.192619759     A.U. after   11 cycles
             Convg  =    0.9056D-08             -V/T =  2.0094
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6          -0.000006626   -0.000002649    0.000002895
      2          6          -0.000010740   -0.000001728    0.000005099
      3          1           0.000000984    0.000008961   -0.000005288
      4          6          -0.000013105   -0.000004526   -0.000014964
      5          6           0.000003339   -0.000002485   -0.000039068
      6          1          -0.000000519    0.000007121   -0.000003314
      7          6           0.000016878   -0.000005547   -0.000009187
      8          6          -0.000002123   -0.000016578    0.000004581
```

9	6	-0.000001841	0.000014710	0.000013215
10	6	-0.000016162	-0.000004965	0.000012619
11	1	-0.000005817	-0.000003679	-0.000005712
12	6	0.000000690	0.000000734	-0.000013614
13	1	0.000003493	0.000004183	-0.000003698
14	6	-0.000001989	-0.000000650	0.000013190
15	1	0.000003835	0.000000344	0.000003147
16	6	-0.000002372	0.000015412	0.000017398
17	1	0.000000835	0.000006327	0.000006020
18	6	-0.000003596	0.000019711	-0.000012340
19	1	0.000001338	0.000008748	0.000001772
20	6	-0.000007135	-0.000002256	-0.000021555
21	1	0.000000832	0.000004121	-0.000004904
22	6	0.000018117	-0.000001394	-0.000001390
23	1	0.000005839	-0.000004391	-0.000000624
24	6	0.000020872	-0.000000684	0.000007005
25	1	0.000005837	-0.000005734	0.000002043
26	6	0.000007761	-0.000012268	0.000025188
27	1	0.000005029	-0.000007729	-0.000003038
28	6	-0.000019291	0.000015087	0.000080690
29	6	0.000046343	-0.000009489	0.000067760
30	8	-0.000009097	0.000009908	-0.000075857
31	8	-0.000007526	0.000001455	-0.000002783
32	8	-0.000009524	-0.000001383	-0.000053825
33	6	-0.000009049	-0.000013209	-0.000005611
34	1	-0.000001458	-0.000007743	0.000001673
35	1	-0.000007263	-0.000004461	0.000015538
36	1	-0.000006793	-0.000003273	-0.000003061

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000080690 RMS     0.000017147


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000057779 RMS     0.000009283
 Search for a local minimum.
 Step number   6 out of a maximum of  216
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6
 DE=  4.26D-07 DEPred=-8.75D-07 R=-4.87D-01
 Trust test=-4.87D-01 RLast= 7.68D-03 DXMaxT set to 5.00D-02
     Eigenvalues ---    0.00401   0.00467   0.01031   0.01143
0.01163
     Eigenvalues ---    0.01431   0.01496   0.01561   0.01789
0.02061
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02110   0.02114   0.02129   0.02130
0.02131
     Eigenvalues ---    0.02134   0.02139   0.02147   0.02155
0.02158
     Eigenvalues ---    0.02167   0.02181   0.02753   0.03865
0.04000
     Eigenvalues ---    0.04595   0.04769   0.05194   0.05322
0.05426
     Eigenvalues ---    0.05496   0.05548   0.05609   0.05932
0.06488
     Eigenvalues ---    0.08254   0.08687   0.09466   0.10153
0.12704
     Eigenvalues ---    0.15775   0.15982   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16019
     Eigenvalues ---    0.16089   0.16819   0.20412   0.21417
0.21999
     Eigenvalues ---    0.22001   0.22354   0.22567   0.22644
0.24073
     Eigenvalues ---    0.24574   0.24648   0.24814   0.25106
0.26469
     Eigenvalues ---    0.27535   0.28055   0.28463   0.28879
0.29125
     Eigenvalues ---    0.29735   0.30220   0.34209   0.34221
0.34259
     Eigenvalues ---    0.34323   0.34512   0.34691   0.35105
0.35154
     Eigenvalues ---    0.35209   0.35218   0.35226   0.35293
0.35339
     Eigenvalues ---    0.35342   0.36555   0.39740   0.42007
0.42039
     Eigenvalues ---    0.42487   0.43775   0.44256   0.45091
0.46033
     Eigenvalues ---    0.46161   0.46363   0.46488   0.46855
0.50866
     Eigenvalues ---    1.04217
1.049831000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     6    5    4    3
2
 RFO step:  Lambda=-3.32125902D-08.
 DIIS coeffs:      0.77826      0.09375      0.12851      0.00132
-0.00183
 Iteration  1 RMS(Cart)=  0.00019198 RMS(Int)=  0.00000003
 Iteration  2 RMS(Cart)=  0.00000002 RMS(Int)=  0.00000002
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86498   0.00001  -0.00001   0.00005   0.00004
2.86502
```

This journal is © The Royal Society of Chemistry 2014

R2	2.65957	0.00001	0.00005	-0.00003	0.00002
2.65959					
R3	2.63114	0.00002	0.00004	0.00000	0.00004
2.63118					
R4	2.06526	0.00001	0.00001	0.00000	0.00001
2.06527					
R5	2.96382	0.00000	0.00005	-0.00005	0.00000
2.96381					
R6	2.86722	0.00000	-0.00001	-0.00002	-0.00003
2.86719					
R7	2.90575	0.00003	0.00001	0.00008	0.00009
2.90585					
R8	2.63557	0.00004	0.00005	0.00001	0.00006
2.63563					
R9	2.06866	0.00000	0.00000	0.00000	0.00000
2.06865					
R10	2.91510	0.00003	-0.00001	0.00009	0.00008
2.91518					
R11	2.87058	0.00000	0.00004	-0.00006	-0.00001
2.87057					
R12	2.66046	0.00002	0.00002	0.00000	0.00002
2.66048					
R13	2.63278	0.00002	0.00002	0.00001	0.00004
2.63281					
R14	2.89933	0.00002	0.00004	0.00003	0.00006
2.89940					
R15	2.63605	0.00002	0.00003	0.00002	0.00004
2.63609					
R16	3.00439	0.00000	-0.00001	0.00002	0.00001
3.00440					
R17	2.88786	0.00001	0.00003	-0.00001	0.00002
2.88788					
R18	2.06971	0.00000	0.00001	-0.00001	0.00000
2.06971					
R19	2.88164	-0.00001	0.00005	-0.00011	-0.00006
2.88158					
R20	2.05525	0.00001	0.00001	0.00000	0.00001
2.05526					
R21	2.64576	0.00002	0.00004	-0.00001	0.00003
2.64579					
R22	2.05197	0.00000	0.00001	-0.00001	0.00000
2.05197					
R23	2.64762	0.00003	0.00004	0.00000	0.00004
2.64766					
R24	2.05383	0.00001	0.00001	0.00000	0.00001
2.05384					
R25	2.63860	0.00003	0.00004	0.00001	0.00004
2.63865					
R26	2.05365	0.00001	0.00001	0.00000	0.00001
2.05366					
R27	2.05600	0.00001	0.00001	0.00000	0.00001
2.05601					

This journal is © The Royal Society of Chemistry 2014

R28	2.64757	0.00003	0.00004	0.00001	0.00005
2.64762					
R29	2.05382	0.00001	0.00001	0.00000	0.00001
2.05383					
R30	2.63754	0.00002	0.00003	-0.00001	0.00003
2.63757					
R31	2.05401	0.00001	0.00001	0.00001	0.00001
2.05402					
R32	2.64956	0.00003	0.00003	0.00001	0.00005
2.64961					
R33	2.05203	0.00000	0.00000	-0.00001	0.00000
2.05202					
R34	2.62417	-0.00003	0.00004	-0.00010	-0.00006
2.62411					
R35	2.26582	0.00005	0.00001	0.00004	0.00005
2.26587					
R36	2.62956	0.00006	-0.00003	0.00016	0.00013
2.62969					
R37	2.26639	0.00000	0.00002	-0.00002	0.00000
2.26639					
R38	2.07047	0.00000	0.00001	0.00000	0.00001
2.07048					
R39	2.06419	0.00001	0.00001	0.00002	0.00003
2.06422					
R40	2.07042	0.00000	0.00000	-0.00001	-0.00001
2.07041					
A1	1.97975	0.00000	0.00001	-0.00001	0.00001
1.97976					
A2	2.19555	-0.00001	-0.00001	-0.00001	-0.00002
2.19553					
A3	2.10782	0.00000	0.00000	0.00002	0.00001
2.10783					
A4	1.97422	0.00000	0.00002	-0.00005	-0.00003
1.97420					
A5	1.83239	0.00000	0.00000	0.00003	0.00003
1.83242					
A6	1.88054	0.00000	0.00001	-0.00002	-0.00002
1.88053					
A7	1.92870	0.00000	0.00001	0.00002	0.00003
1.92873					
A8	1.96670	0.00000	-0.00001	-0.00002	-0.00004
1.96666					
A9	1.87371	0.00000	-0.00003	0.00005	0.00002
1.87374					
A10	1.99424	0.00000	-0.00001	-0.00001	-0.00002
1.99422					
A11	2.08538	-0.00001	-0.00002	0.00000	-0.00002
2.08536					
A12	2.20357	0.00001	0.00003	0.00001	0.00003
2.20360					
A13	1.90074	0.00000	-0.00005	0.00001	-0.00003
1.90071					

This journal is © The Royal Society of Chemistry 2014

A14	1.91633	0.00000	0.00001	-0.00001	0.00000
1.91633					
A15	1.96295	0.00000	0.00003	0.00003	0.00007
1.96302					
A16	1.96860	0.00000	0.00002	-0.00001	0.00000
1.96860					
A17	1.88611	0.00000	-0.00001	0.00002	0.00001
1.88612					
A18	1.82932	0.00000	0.00000	-0.00004	-0.00004
1.82928					
A19	1.98493	0.00000	0.00000	0.00000	-0.00001
1.98492					
A20	2.19263	-0.00001	-0.00001	-0.00002	-0.00002
2.19261					
A21	2.10561	0.00001	0.00001	0.00002	0.00003
2.10564					
A22	1.98940	0.00000	0.00001	0.00000	0.00002
1.98942					
A23	2.08813	-0.00001	-0.00001	-0.00003	-0.00004
2.08809					
A24	2.20555	0.00001	0.00000	0.00003	0.00002
2.20557					
A25	1.85763	0.00000	0.00002	-0.00001	0.00001
1.85763					
A26	1.81551	0.00000	-0.00004	-0.00004	-0.00009
1.81542					
A27	1.98618	0.00001	0.00007	-0.00001	0.00006
1.98624					
A28	1.84318	0.00000	0.00001	0.00004	0.00005
1.84324					
A29	1.99834	0.00000	0.00000	0.00001	0.00001
1.99836					
A30	1.94805	-0.00001	-0.00005	0.00000	-0.00006
1.94800					
A31	1.93613	0.00000	0.00001	-0.00001	-0.00001
1.93613					
A32	1.96417	0.00000	-0.00001	-0.00001	-0.00002
1.96415					
A33	1.81387	0.00001	0.00002	0.00002	0.00004
1.81392					
A34	1.88368	0.00000	0.00002	-0.00001	0.00001
1.88370					
A35	1.98912	0.00000	0.00002	-0.00004	-0.00002
1.98910					
A36	1.87744	-0.00001	-0.00007	0.00005	-0.00002
1.87742					
A37	2.09633	0.00000	0.00000	-0.00001	-0.00001
2.09633					
A38	2.08546	0.00000	0.00000	0.00000	0.00000
2.08547					
A39	2.10139	0.00000	0.00000	0.00001	0.00000
2.10139					

This journal is © The Royal Society of Chemistry 2014

A40	2.10591	0.00000	-0.00001	0.00001	0.00000
2.10590					
A41	2.08924	0.00000	0.00001	0.00001	0.00002
2.08926					
A42	2.08803	0.00000	0.00000	-0.00002	-0.00002
2.08801					
A43	2.08687	0.00000	0.00000	0.00000	0.00001
2.08688					
A44	2.10227	0.00000	-0.00001	0.00001	0.00000
2.10227					
A45	2.09404	0.00000	0.00000	-0.00001	-0.00001
2.09403					
A46	2.09560	0.00000	-0.00001	-0.00001	-0.00002
2.09558					
A47	2.09167	0.00000	0.00000	0.00002	0.00001
2.09168					
A48	2.09591	0.00000	0.00001	0.00000	0.00000
2.09591					
A49	2.09718	0.00000	-0.00001	0.00002	0.00001
2.09718					
A50	2.08594	0.00000	0.00001	-0.00002	0.00000
2.08594					
A51	2.10005	0.00000	0.00000	0.00000	-0.00001
2.10004					
A52	2.09264	0.00000	0.00000	0.00000	0.00001
2.09265					
A53	2.09401	0.00000	0.00000	0.00001	0.00000
2.09401					
A54	2.09653	0.00000	0.00000	-0.00001	-0.00001
2.09652					
A55	2.09428	0.00000	0.00000	0.00000	0.00000
2.09427					
A56	2.10210	0.00000	-0.00001	0.00000	-0.00001
2.10210					
A57	2.08680	0.00000	0.00001	0.00000	0.00001
2.08681					
A58	2.09108	0.00000	0.00002	-0.00001	0.00001
2.09109					
A59	2.10727	0.00000	0.00001	0.00001	0.00003
2.10730					
A60	2.08481	-0.00001	-0.00003	-0.00001	-0.00004
2.08477					
A61	1.91575	0.00001	-0.00003	0.00006	0.00003
1.91578					
A62	2.24618	-0.00002	0.00005	-0.00011	-0.00007
2.24612					
A63	2.12125	0.00001	-0.00002	0.00005	0.00003
2.12128					
A64	1.91976	-0.00002	-0.00003	-0.00002	-0.00005
1.91971					
A65	2.25466	0.00001	0.00000	0.00005	0.00005
2.25471					

```
   A66        2.10855   0.00000   0.00003  -0.00003   0.00000
2.10855
   A67        1.94601   0.00001   0.00004  -0.00003   0.00001
1.94602
   A68        1.93275   0.00000  -0.00002   0.00004   0.00002
1.93277
   A69        1.94187   0.00002   0.00003   0.00006   0.00010
1.94197
   A70        1.93296  -0.00001  -0.00003  -0.00001  -0.00004
1.93292
   A71        1.87373  -0.00001   0.00001  -0.00006  -0.00004
1.87369
   A72        1.88558   0.00000   0.00001   0.00000   0.00001
1.88559
   A73        1.89488  -0.00001  -0.00001  -0.00004  -0.00005
1.89482
    D1        3.12750   0.00000   0.00000  -0.00003  -0.00003
3.12747
    D2       -1.05136   0.00000   0.00003  -0.00001   0.00002  -
1.05134
    D3        0.94182   0.00000   0.00000   0.00005   0.00005
0.94187
    D4       -0.02567   0.00000   0.00008  -0.00006   0.00002  -
0.02565
    D5        2.07866   0.00000   0.00010  -0.00004   0.00006
2.07872
    D6       -2.21135   0.00000   0.00007   0.00002   0.00010  -
2.21125
    D7       -0.00743   0.00000   0.00000  -0.00001  -0.00001  -
0.00744
    D8        3.13230   0.00000   0.00000  -0.00006  -0.00006
3.13224
    D9       -3.13810   0.00000  -0.00007   0.00001  -0.00006  -
3.13815
   D10        0.00163   0.00000  -0.00007  -0.00003  -0.00010
0.00153
   D11        0.01202   0.00000  -0.00002   0.00005   0.00003
0.01205
   D12       -3.13587   0.00000  -0.00005   0.00002  -0.00003  -
3.13590
   D13        3.14126   0.00000   0.00006   0.00002   0.00008
3.14133
   D14       -0.00664   0.00000   0.00003  -0.00001   0.00002  -
0.00662
   D15       -1.13320   0.00000  -0.00010  -0.00003  -0.00013  -
1.13333
   D16        1.03015   0.00000  -0.00010  -0.00005  -0.00015
1.03000
   D17        3.05979   0.00000  -0.00008  -0.00008  -0.00016
3.05963
   D18        1.00095   0.00000  -0.00006  -0.00006  -0.00013
1.00082
```

This journal is © The Royal Society of Chemistry 2014

D19	-3.11888	0.00000	-0.00007	-0.00008	-0.00015	-3.11903
D20	-1.08924	0.00000	-0.00004	-0.00011	-0.00016	-1.08940
D21	-3.13115	0.00000	-0.00009	-0.00004	-0.00014	-3.13129
D22	-0.96780	0.00000	-0.00010	-0.00006	-0.00016	-0.96796
D23	1.06184	0.00000	-0.00007	-0.00009	-0.00017	1.06167
D24	-0.93453	-0.00001	-0.00003	-0.00008	-0.00011	-0.93463
D25	2.21396	0.00000	-0.00001	-0.00011	-0.00011	2.21385
D26	-3.12469	0.00000	-0.00005	0.00001	-0.00004	-3.12472
D27	0.02381	0.00000	-0.00003	-0.00001	-0.00004	0.02377
D28	1.03096	0.00000	-0.00003	-0.00004	-0.00007	1.03089
D29	-2.10373	0.00000	-0.00001	-0.00006	-0.00008	-2.10381
D30	-0.91648	0.00000	0.00004	0.00001	0.00005	-0.91643
D31	1.02554	0.00000	0.00003	0.00004	0.00007	1.02562
D32	-3.13400	0.00000	-0.00002	0.00001	-0.00002	-3.13402
D33	2.22712	0.00000	0.00004	0.00006	0.00010	2.22722
D34	-2.11404	0.00000	0.00003	0.00009	0.00012	-2.11391
D35	0.00960	0.00000	-0.00003	0.00006	0.00003	0.00964
D36	0.00444	0.00000	0.00006	0.00007	0.00013	0.00457
D37	3.13893	0.00000	0.00004	0.00003	0.00007	3.13900
D38	-3.13926	0.00000	0.00006	0.00001	0.00008	-3.13918
D39	-0.00477	0.00000	0.00005	-0.00003	0.00002	-0.00475
D40	-0.02663	0.00000	0.00013	0.00011	0.00024	-0.02639
D41	-2.13908	0.00000	0.00011	0.00013	0.00024	-2.13884
D42	2.11812	0.00000	0.00018	0.00006	0.00024	2.11837
D43	2.09661	0.00000	0.00009	0.00010	0.00020	2.09681
D44	-0.01583	0.00000	0.00007	0.00013	0.00020	-0.01563

This journal is © The Royal Society of Chemistry 2014

D45	-2.04182	0.00000	0.00014	0.00006	0.00020	-2.04161
D46	-2.13884	0.00000	0.00009	0.00009	0.00018	-2.13865
D47	2.03190	0.00000	0.00006	0.00012	0.00018	2.03209
D48	0.00592	0.00000	0.00013	0.00005	0.00019	0.00610
D49	-2.08099	0.00000	-0.00019	0.00012	-0.00007	-2.08106
D50	1.06524	0.00000	-0.00010	0.00017	0.00007	1.06531
D51	2.10353	0.00000	-0.00015	0.00007	-0.00008	2.10345
D52	-1.03343	0.00000	-0.00006	0.00012	0.00006	-1.03337
D53	0.00016	0.00000	-0.00016	0.00010	-0.00006	0.00010
D54	-3.13680	0.00000	-0.00007	0.00015	0.00008	-3.13672
D55	-0.00971	0.00000	0.00006	0.00007	0.00013	-0.00958
D56	-3.13642	0.00000	0.00000	-0.00007	-0.00007	-3.13650
D57	3.12537	0.00000	0.00004	0.00009	0.00013	3.12550
D58	-0.00135	0.00000	-0.00002	-0.00005	-0.00007	-0.00142
D59	0.00386	0.00000	-0.00004	0.00008	0.00004	0.00390
D60	-3.14005	0.00000	0.00001	0.00007	0.00008	-3.13997
D61	-3.13039	0.00000	-0.00002	0.00005	0.00004	-3.13035
D62	0.00888	0.00000	0.00003	0.00005	0.00008	0.00896
D63	0.92396	0.00000	-0.00006	-0.00004	-0.00010	0.92386
D64	-0.99872	0.00000	-0.00002	-0.00001	-0.00003	-0.99874
D65	3.13419	0.00001	0.00004	-0.00004	0.00000	3.13419
D66	-2.23369	0.00000	0.00000	0.00011	0.00012	-2.23357
D67	2.12682	0.00000	0.00004	0.00015	0.00019	2.12701
D68	-0.02345	0.00001	0.00011	0.00011	0.00022	-0.02324
D69	3.13131	0.00000	0.00006	0.00004	0.00010	3.13142
D70	-0.00728	0.00000	0.00000	0.00001	0.00001	-0.00727

This journal is © The Royal Society of Chemistry 2014

D71	0.00660	0.00000	0.00000	-0.00012	-0.00013	0.00647
D72	-3.13200	0.00000	-0.00007	-0.00015	-0.00022	-3.13221
D73	-0.96676	0.00000	-0.00011	-0.00009	-0.00020	-0.96696
D74	1.19250	0.00000	-0.00010	-0.00012	-0.00022	1.19227
D75	-3.00663	-0.00001	-0.00016	-0.00009	-0.00024	-3.00688
D76	0.98576	0.00000	-0.00011	-0.00010	-0.00021	0.98555
D77	-3.13817	0.00000	-0.00010	-0.00013	-0.00023	-3.13840
D78	-1.05411	-0.00001	-0.00015	-0.00010	-0.00025	-1.05437
D79	-3.11554	0.00000	-0.00013	-0.00006	-0.00019	-3.11574
D80	-0.95629	0.00000	-0.00013	-0.00008	-0.00021	-0.95650
D81	1.12777	-0.00001	-0.00018	-0.00005	-0.00024	1.12753
D82	-1.03009	0.00000	0.00012	0.00012	0.00024	-1.02985
D83	-3.11253	0.00000	0.00010	0.00012	0.00022	-3.11231
D84	1.06140	0.00000	0.00011	0.00014	0.00025	1.06165
D85	3.11097	0.00000	0.00005	0.00012	0.00017	3.11113
D86	1.02852	0.00000	0.00002	0.00012	0.00014	1.02866
D87	-1.08073	0.00000	0.00003	0.00014	0.00017	-1.08056
D88	1.01824	0.00000	0.00008	0.00005	0.00013	1.01837
D89	-1.06421	0.00000	0.00005	0.00006	0.00011	-1.06410
D90	3.10972	0.00000	0.00006	0.00007	0.00014	3.10986
D91	-0.01037	0.00000	-0.00007	-0.00019	-0.00026	-0.01064
D92	3.10872	0.00000	0.00004	-0.00022	-0.00018	3.10854
D93	2.09917	0.00000	-0.00004	-0.00022	-0.00025	2.09892
D94	-1.06492	0.00000	0.00008	-0.00025	-0.00017	-1.06509
D95	-2.09643	0.00000	-0.00004	-0.00022	-0.00026	-2.09668
D96	1.02267	0.00000	0.00007	-0.00025	-0.00018	1.02249

This journal is © The Royal Society of Chemistry 2014

D97	-0.00777	0.00000	-0.00002	-0.00001	-0.00004	-0.00780
D98	3.13789	0.00000	0.00000	-0.00004	-0.00004	3.13785
D99	3.13150	0.00000	0.00002	-0.00002	0.00001	3.13150
D100	-0.00604	0.00000	0.00005	-0.00005	0.00000	-0.00603
D101	-3.13778	0.00000	0.00000	0.00003	0.00003	-3.13775
D102	0.00840	0.00000	0.00001	0.00002	0.00003	0.00844
D103	0.00678	0.00000	-0.00006	0.00001	-0.00006	0.00672
D104	-3.13022	0.00000	-0.00005	-0.00001	-0.00006	-3.13028
D105	-0.00084	0.00000	0.00000	-0.00002	-0.00002	-0.00086
D106	3.13668	0.00000	-0.00002	0.00001	-0.00002	3.13666
D107	-3.13783	0.00000	0.00001	-0.00003	-0.00002	-3.13785
D108	-0.00030	0.00000	-0.00002	0.00000	-0.00002	-0.00032
D109	-3.13340	0.00000	-0.00002	0.00003	0.00001	-3.13338
D110	0.00557	0.00000	0.00001	0.00002	0.00003	0.00560
D111	0.00188	0.00000	-0.00005	0.00001	-0.00004	0.00184
D112	3.14085	0.00000	-0.00002	-0.00001	-0.00003	3.14082
D113	-3.13881	0.00000	-0.00002	0.00000	-0.00002	-3.13883
D114	0.00047	0.00000	-0.00001	0.00002	0.00000	0.00047
D115	0.00015	0.00000	0.00001	-0.00002	0.00000	0.00015
D116	3.13943	0.00000	0.00002	0.00000	0.00001	3.13945
D117	-0.00551	0.00000	-0.00002	-0.00006	-0.00008	-0.00558
D118	-3.14008	0.00000	0.00000	-0.00002	-0.00002	-3.14011
D119	3.13379	0.00000	-0.00002	-0.00004	-0.00006	3.13372
D120	-0.00079	0.00000	0.00000	-0.00001	-0.00001	-0.00080
D121	-0.00704	0.00000	0.00012	-0.00023	-0.00011	-0.00716
D122	3.13031	0.00000	0.00004	-0.00028	-0.00024	3.13007

This journal is © The Royal Society of Chemistry 2014

```
   D123       0.01116   0.00000  -0.00003   0.00027   0.00024
0.01140
   D124      -3.11013   0.00000  -0.00013   0.00030   0.00017  -
3.10996
         Item               Value     Threshold  Converged?
 Maximum Force            0.000058     0.000450     YES
 RMS     Force            0.000009     0.000300     YES
 Maximum Displacement     0.001367     0.001800     YES
 RMS     Displacement     0.000192     0.001200     YES
 Predicted change in Energy=-3.611031D-08
 Optimization completed.
    -- Stationary point found.
                           ----------------------------
                           !   Optimized Parameters   !
                           ! (Angstroms and Degrees)  !
 --------------------------                            ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ---------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.5161         -DE/DX =    0.0
!
 ! R2    R(1,4)                  1.4074         -DE/DX =    0.0
!
 ! R3    R(1,20)                 1.3923         -DE/DX =    0.0
!
 ! R4    R(2,3)                  1.0929         -DE/DX =    0.0
!
 ! R5    R(2,5)                  1.5684         -DE/DX =    0.0
!
 ! R6    R(2,7)                  1.5173         -DE/DX =    0.0
!
 ! R7    R(4,9)                  1.5377         -DE/DX =    0.0
!
 ! R8    R(4,26)                 1.3947         -DE/DX =    0.0
!
 ! R9    R(5,6)                  1.0947         -DE/DX =    0.0
!
 ! R10   R(5,10)                 1.5426         -DE/DX =    0.0
!
 ! R11   R(5,28)                 1.519          -DE/DX =    0.0
!
 ! R12   R(7,8)                  1.4079         -DE/DX =    0.0
!
 ! R13   R(7,12)                 1.3932         -DE/DX =    0.0
!
 ! R14   R(8,9)                  1.5343         -DE/DX =    0.0
!
 ! R15   R(8,14)                 1.3949         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R16   R(9,10)                1.5899         -DE/DX =    0.0
!
 ! R17   R(9,33)                1.5282         -DE/DX =    0.0
!
 ! R18   R(10,11)               1.0952         -DE/DX =    0.0
!
 ! R19   R(10,29)               1.5249         -DE/DX =    0.0
!
 ! R20   R(12,13)               1.0876         -DE/DX =    0.0
!
 ! R21   R(12,18)               1.4001         -DE/DX =    0.0
!
 ! R22   R(14,15)               1.0859         -DE/DX =    0.0
!
 ! R23   R(14,16)               1.4011         -DE/DX =    0.0
!
 ! R24   R(16,17)               1.0868         -DE/DX =    0.0
!
 ! R25   R(16,18)               1.3963         -DE/DX =    0.0
!
 ! R26   R(18,19)               1.0867         -DE/DX =    0.0
!
 ! R27   R(20,21)               1.088          -DE/DX =    0.0
!
 ! R28   R(20,22)               1.401          -DE/DX =    0.0
!
 ! R29   R(22,23)               1.0868         -DE/DX =    0.0
!
 ! R30   R(22,24)               1.3957         -DE/DX =    0.0
!
 ! R31   R(24,25)               1.0869         -DE/DX =    0.0
!
 ! R32   R(24,26)               1.4021         -DE/DX =    0.0
!
 ! R33   R(26,27)               1.0859         -DE/DX =    0.0
!
 ! R34   R(28,30)               1.3887         -DE/DX =    0.0
!
 ! R35   R(28,32)               1.199          -DE/DX =    0.0
!
 ! R36   R(29,30)               1.3915         -DE/DX =    0.0001
!
 ! R37   R(29,31)               1.1993         -DE/DX =    0.0
!
 ! R38   R(33,34)               1.0956         -DE/DX =    0.0
!
 ! R39   R(33,35)               1.0923         -DE/DX =    0.0
!
 ! R40   R(33,36)               1.0956         -DE/DX =    0.0
!
 ! A1    A(2,1,4)             113.4314         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A2    A(2,1,20)            125.796          -DE/DX =    0.0
!
 ! A3    A(4,1,20)            120.7693         -DE/DX =    0.0
!
 ! A4    A(1,2,3)             113.1147         -DE/DX =    0.0
!
 ! A5    A(1,2,5)             104.9883         -DE/DX =    0.0
!
 ! A6    A(1,2,7)             107.7471         -DE/DX =    0.0
!
 ! A7    A(3,2,5)             110.5063         -DE/DX =    0.0
!
 ! A8    A(3,2,7)             112.6836         -DE/DX =    0.0
!
 ! A9    A(5,2,7)             107.3559         -DE/DX =    0.0
!
 ! A10   A(1,4,9)             114.2614         -DE/DX =    0.0
!
 ! A11   A(1,4,26)            119.4835         -DE/DX =    0.0
!
 ! A12   A(9,4,26)            126.255          -DE/DX =    0.0
!
 ! A13   A(2,5,6)             108.9045         -DE/DX =    0.0
!
 ! A14   A(2,5,10)            109.7977         -DE/DX =    0.0
!
 ! A15   A(2,5,28)            112.4688         -DE/DX =    0.0
!
 ! A16   A(6,5,10)            112.7924         -DE/DX =    0.0
!
 ! A17   A(6,5,28)            108.0661         -DE/DX =    0.0
!
 ! A18   A(10,5,28)           104.8123         -DE/DX =    0.0
!
 ! A19   A(2,7,8)             113.7281         -DE/DX =    0.0
!
 ! A20   A(2,7,12)            125.6283         -DE/DX =    0.0
!
 ! A21   A(8,7,12)            120.6424         -DE/DX =    0.0
!
 ! A22   A(7,8,9)             113.9844         -DE/DX =    0.0
!
 ! A23   A(7,8,14)            119.6408         -DE/DX =    0.0
!
 ! A24   A(9,8,14)            126.3686         -DE/DX =    0.0
!
 ! A25   A(4,9,8)             106.4341         -DE/DX =    0.0
!
 ! A26   A(4,9,10)            104.0212         -DE/DX =    0.0
!
 ! A27   A(4,9,33)            113.7996         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A28   A(8,9,10)            105.6067         -DE/DX =    0.0
!
 ! A29   A(8,9,33)            114.4967         -DE/DX =    0.0
!
 ! A30   A(10,9,33)           111.6153         -DE/DX =    0.0
!
 ! A31   A(5,10,9)            110.9322         -DE/DX =    0.0
!
 ! A32   A(5,10,11)           112.5388         -DE/DX =    0.0
!
 ! A33   A(5,10,29)           103.9272         -DE/DX =    0.0
!
 ! A34   A(9,10,11)           107.927          -DE/DX =    0.0
!
 ! A35   A(9,10,29)           113.9681         -DE/DX =    0.0
!
 ! A36   A(11,10,29)          107.5692         -DE/DX =    0.0
!
 ! A37   A(7,12,13)           120.111          -DE/DX =    0.0
!
 ! A38   A(7,12,18)           119.4883         -DE/DX =    0.0
!
 ! A39   A(13,12,18)          120.4007         -DE/DX =    0.0
!
 ! A40   A(8,14,15)           120.6595         -DE/DX =    0.0
!
 ! A41   A(8,14,16)           119.7049         -DE/DX =    0.0
!
 ! A42   A(15,14,16)          119.6354         -DE/DX =    0.0
!
 ! A43   A(14,16,17)          119.5689         -DE/DX =    0.0
!
 ! A44   A(14,16,18)          120.4512         -DE/DX =    0.0
!
 ! A45   A(17,16,18)          119.9794         -DE/DX =    0.0
!
 ! A46   A(12,18,16)          120.0691         -DE/DX =    0.0
!
 ! A47   A(12,18,19)          119.8437         -DE/DX =    0.0
!
 ! A48   A(16,18,19)          120.0867         -DE/DX =    0.0
!
 ! A49   A(1,20,21)           120.1594         -DE/DX =    0.0
!
 ! A50   A(1,20,22)           119.5158         -DE/DX =    0.0
!
 ! A51   A(21,20,22)          120.3239         -DE/DX =    0.0
!
 ! A52   A(20,22,23)          119.8993         -DE/DX =    0.0
!
 ! A53   A(20,22,24)          119.9781         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A54   A(23,22,24)          120.1225         -DE/DX =    0.0
!
 ! A55   A(22,24,25)          119.9933         -DE/DX =    0.0
!
 ! A56   A(22,24,26)          120.4416         -DE/DX =    0.0
!
 ! A57   A(25,24,26)          119.565          -DE/DX =    0.0
!
 ! A58   A(4,26,24)           119.8103         -DE/DX =    0.0
!
 ! A59   A(4,26,27)           120.738          -DE/DX =    0.0
!
 ! A60   A(24,26,27)          119.4505         -DE/DX =    0.0
!
 ! A61   A(5,28,30)           109.7641         -DE/DX =    0.0
!
 ! A62   A(5,28,32)           128.6967         -DE/DX =    0.0
!
 ! A63   A(30,28,32)          121.5386         -DE/DX =    0.0
!
 ! A64   A(10,29,30)          109.9944         -DE/DX =    0.0
!
 ! A65   A(10,29,31)          129.1824         -DE/DX =    0.0
!
 ! A66   A(30,29,31)          120.811          -DE/DX =    0.0
!
 ! A67   A(28,30,29)          111.4982         -DE/DX =    0.0
!
 ! A68   A(9,33,34)           110.7384         -DE/DX =    0.0
!
 ! A69   A(9,33,35)           111.2611         -DE/DX =    0.0
!
 ! A70   A(9,33,36)           110.7502         -DE/DX =    0.0
!
 ! A71   A(34,33,35)          107.3568         -DE/DX =    0.0
!
 ! A72   A(34,33,36)          108.0358         -DE/DX =    0.0
!
 ! A73   A(35,33,36)          108.5684         -DE/DX =    0.0
!
 ! D1    D(4,1,2,3)           179.1924         -DE/DX =    0.0
!
 ! D2    D(4,1,2,5)           -60.2383         -DE/DX =    0.0
!
 ! D3    D(4,1,2,7)            53.9621         -DE/DX =    0.0
!
 ! D4    D(20,1,2,3)           -1.4708         -DE/DX =    0.0
!
 ! D5    D(20,1,2,5)          119.0985         -DE/DX =    0.0
!
 ! D6    D(20,1,2,7)         -126.7011         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D7    D(2,1,4,9)              -0.4257         -DE/DX =    0.0
!
 ! D8    D(2,1,4,26)            179.4674         -DE/DX =    0.0
!
 ! D9    D(20,1,4,9)           -179.7997         -DE/DX =    0.0
!
 ! D10   D(20,1,4,26)            0.0935         -DE/DX =    0.0
!
 ! D11   D(2,1,20,21)            0.6889         -DE/DX =    0.0
!
 ! D12   D(2,1,20,22)          -179.6724         -DE/DX =    0.0
!
 ! D13   D(4,1,20,21)           179.9807         -DE/DX =    0.0
!
 ! D14   D(4,1,20,22)            -0.3806         -DE/DX =    0.0
!
 ! D15   D(1,2,5,6)             -64.9278         -DE/DX =    0.0
!
 ! D16   D(1,2,5,10)             59.0231         -DE/DX =    0.0
!
 ! D17   D(1,2,5,28)            175.3129         -DE/DX =    0.0
!
 ! D18   D(3,2,5,6)              57.3502         -DE/DX =    0.0
!
 ! D19   D(3,2,5,10)           -178.6988         -DE/DX =    0.0
!
 ! D20   D(3,2,5,28)            -62.4091         -DE/DX =    0.0
!
 ! D21   D(7,2,5,6)            -179.4017         -DE/DX =    0.0
!
 ! D22   D(7,2,5,10)            -55.4508         -DE/DX =    0.0
!
 ! D23   D(7,2,5,28)             60.839          -DE/DX =    0.0
!
 ! D24   D(1,2,7,8)              -53.5444         -DE/DX =    0.0
!
 ! D25   D(1,2,7,12)            126.8508         -DE/DX =    0.0
!
 ! D26   D(3,2,7,8)            -179.0313         -DE/DX =    0.0
!
 ! D27   D(3,2,7,12)              1.364          -DE/DX =    0.0
!
 ! D28   D(5,2,7,8)              59.0698         -DE/DX =    0.0
!
 ! D29   D(5,2,7,12)           -120.535          -DE/DX =    0.0
!
 ! D30   D(1,4,9,8)              -52.5107         -DE/DX =    0.0
!
 ! D31   D(1,4,9,10)             58.7593         -DE/DX =    0.0
!
 ! D32   D(1,4,9,33)           -179.565          -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D33   D(26,4,9,8)          127.6046         -DE/DX =    0.0
!
 ! D34   D(26,4,9,10)        -121.1254         -DE/DX =    0.0
!
 ! D35   D(26,4,9,33)           0.5503         -DE/DX =    0.0
!
 ! D36   D(1,4,26,24)           0.2545         -DE/DX =    0.0
!
 ! D37   D(1,4,26,27)         179.8473         -DE/DX =    0.0
!
 ! D38   D(9,4,26,24)        -179.8663         -DE/DX =    0.0
!
 ! D39   D(9,4,26,27)           -0.2735         -DE/DX =    0.0
!
 ! D40   D(2,5,10,9)            -1.5259         -DE/DX =    0.0
!
 ! D41   D(2,5,10,11)         -122.5602         -DE/DX =    0.0
!
 ! D42   D(2,5,10,29)          121.3594         -DE/DX =    0.0
!
 ! D43   D(6,5,10,9)           120.1271         -DE/DX =    0.0
!
 ! D44   D(6,5,10,11)           -0.9072         -DE/DX =    0.0
!
 ! D45   D(6,5,10,29)         -116.9876         -DE/DX =    0.0
!
 ! D46   D(28,5,10,9)         -122.5463         -DE/DX =    0.0
!
 ! D47   D(28,5,10,11)         116.4194         -DE/DX =    0.0
!
 ! D48   D(28,5,10,29)           0.339          -DE/DX =    0.0
!
 ! D49   D(2,5,28,30)         -119.2321         -DE/DX =    0.0
!
 ! D50   D(2,5,28,32)           61.0335         -DE/DX =    0.0
!
 ! D51   D(6,5,28,30)          120.5232         -DE/DX =    0.0
!
 ! D52   D(6,5,28,32)          -59.2113         -DE/DX =    0.0
!
 ! D53   D(10,5,28,30)           0.0092         -DE/DX =    0.0
!
 ! D54   D(10,5,28,32)        -179.7252         -DE/DX =    0.0
!
 ! D55   D(2,7,8,9)             -0.5561         -DE/DX =    0.0
!
 ! D56   D(2,7,8,14)          -179.7039         -DE/DX =    0.0
!
 ! D57   D(12,7,8,9)           179.0705         -DE/DX =    0.0
!
 ! D58   D(12,7,8,14)           -0.0772         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D59   D(2,7,12,13)            0.2213         -DE/DX =    0.0
!
 ! D60   D(2,7,12,18)         -179.9119         -DE/DX =    0.0
!
 ! D61   D(8,7,12,13)         -179.3582         -DE/DX =    0.0
!
 ! D62   D(8,7,12,18)            0.5086         -DE/DX =    0.0
!
 ! D63   D(7,8,9,4)              52.9388         -DE/DX =    0.0
!
 ! D64   D(7,8,9,10)            -57.2223         -DE/DX =    0.0
!
 ! D65   D(7,8,9,33)            179.5761         -DE/DX =    0.0
!
 ! D66   D(14,8,9,4)          -127.9811         -DE/DX =    0.0
!
 ! D67   D(14,8,9,10)           121.8578         -DE/DX =    0.0
!
 ! D68   D(14,8,9,33)            -1.3438         -DE/DX =    0.0
!
 ! D69   D(7,8,14,15)           179.4111         -DE/DX =    0.0
!
 ! D70   D(7,8,14,16)            -0.4173         -DE/DX =    0.0
!
 ! D71   D(9,8,14,15)             0.3781         -DE/DX =    0.0
!
 ! D72   D(9,8,14,16)          -179.4502         -DE/DX =    0.0
!
 ! D73   D(4,9,10,5)            -55.3912         -DE/DX =    0.0
!
 ! D74   D(4,9,10,11)            68.325          -DE/DX =    0.0
!
 ! D75   D(4,9,10,29)          -172.2673         -DE/DX =    0.0
!
 ! D76   D(8,9,10,5)              56.4797         -DE/DX =    0.0
!
 ! D77   D(8,9,10,11)          -179.804          -DE/DX =    0.0
!
 ! D78   D(8,9,10,29)           -60.3963         -DE/DX =    0.0
!
 ! D79   D(33,9,10,5)          -178.5076         -DE/DX =    0.0
!
 ! D80   D(33,9,10,11)          -54.7913         -DE/DX =    0.0
!
 ! D81   D(33,9,10,29)           64.6164         -DE/DX =    0.0
!
 ! D82   D(4,9,33,34)           -59.0196         -DE/DX =    0.0
!
 ! D83   D(4,9,33,35)          -178.3348         -DE/DX =    0.0
!
 ! D84   D(4,9,33,36)            60.8138         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D85   D(8,9,33,34)          178.2452         -DE/DX =    0.0
!
 ! D86   D(8,9,33,35)           58.93           -DE/DX =    0.0
!
 ! D87   D(8,9,33,36)          -61.9214         -DE/DX =    0.0
!
 ! D88   D(10,9,33,34)          58.3407         -DE/DX =    0.0
!
 ! D89   D(10,9,33,35)         -60.9745         -DE/DX =    0.0
!
 ! D90   D(10,9,33,36)         178.1741         -DE/DX =    0.0
!
 ! D91   D(5,10,29,30)          -0.5943         -DE/DX =    0.0
!
 ! D92   D(5,10,29,31)         178.1167         -DE/DX =    0.0
!
 ! D93   D(9,10,29,30)         120.2735         -DE/DX =    0.0
!
 ! D94   D(9,10,29,31)         -61.0154         -DE/DX =    0.0
!
 ! D95   D(11,10,29,30)       -120.1164         -DE/DX =    0.0
!
 ! D96   D(11,10,29,31)         58.5947         -DE/DX =    0.0
!
 ! D97   D(7,12,18,16)          -0.4449         -DE/DX =    0.0
!
 ! D98   D(7,12,18,19)         179.7876         -DE/DX =    0.0
!
 ! D99   D(13,12,18,16)        179.4215         -DE/DX =    0.0
!
 ! D100  D(13,12,18,19)         -0.3459         -DE/DX =    0.0
!
 ! D101  D(8,14,16,17)        -179.7815         -DE/DX =    0.0
!
 ! D102  D(8,14,16,18)           0.4816         -DE/DX =    0.0
!
 ! D103  D(15,14,16,17)          0.3884         -DE/DX =    0.0
!
 ! D104  D(15,14,16,18)       -179.3486         -DE/DX =    0.0
!
 ! D105  D(14,16,18,12)         -0.0483         -DE/DX =    0.0
!
 ! D106  D(14,16,18,19)        179.7186         -DE/DX =    0.0
!
 ! D107  D(17,16,18,12)       -179.7842         -DE/DX =    0.0
!
 ! D108  D(17,16,18,19)         -0.0173         -DE/DX =    0.0
!
 ! D109  D(1,20,22,23)        -179.5304         -DE/DX =    0.0
!
 ! D110  D(1,20,22,24)           0.3192         -DE/DX =    0.0
!
```

```
 ! D111  D(21,20,22,23)          0.1077         -DE/DX =    0.0
!
 ! D112  D(21,20,22,24)        179.9573         -DE/DX =    0.0
!
 ! D113  D(20,22,24,25)       -179.8408         -DE/DX =    0.0
!
 ! D114  D(20,22,24,26)          0.0269         -DE/DX =    0.0
!
 ! D115  D(23,22,24,25)          0.0086         -DE/DX =    0.0
!
 ! D116  D(23,22,24,26)        179.8762         -DE/DX =    0.0
!
 ! D117  D(22,24,26,4)          -0.3155         -DE/DX =    0.0
!
 ! D118  D(22,24,26,27)       -179.9135         -DE/DX =    0.0
!
 ! D119  D(25,24,26,4)         179.5527         -DE/DX =    0.0
!
 ! D120  D(25,24,26,27)         -0.0453         -DE/DX =    0.0
!
 ! D121  D(5,28,30,29)          -0.4034         -DE/DX =    0.0
!
 ! D122  D(32,28,30,29)        179.3534         -DE/DX =    0.0
!
 ! D123  D(10,29,30,28)          0.6393         -DE/DX =    0.0
!
 ! D124  D(31,29,30,28)       -178.1974         -DE/DX =    0.0
!
 ---------------------------------------------------------------------
-----------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.707057   -0.046972   -0.893730
      2          6           0        0.299472   -0.056339   -1.456861
      3          1           0        0.273468    0.001675   -2.547899
      4          6           0        1.747852   -0.103276    0.511935
      5          6           0       -0.325821   -1.407405   -0.963446
      6          1           0        0.220349   -2.238790   -1.420428
      7          6           0       -0.471928    1.068704   -0.792536
      8          6           0       -0.434844    1.027475    0.614225
      9          6           0        0.365070   -0.151892    1.182716
     10          6           0       -0.310567   -1.457948    0.578254
     11          1           0        0.231754   -2.327605    0.964439
     12          6           0       -1.176618    2.071345   -1.455214
     13          1           0       -1.208145    2.088916   -2.542206
```

This journal is © The Royal Society of Chemistry 2014

14	6	0	-1.109177	2.001305	1.350956
15	1	0	-1.099498	1.979872	2.436555
16	6	0	-1.809148	3.015468	0.684264
17	1	0	-2.330801	3.775132	1.260463
18	6	0	-1.844187	3.051591	-0.711118
19	1	0	-2.392748	3.838336	-1.222126
20	6	0	2.882167	-0.002737	-1.639230
21	1	0	2.839061	0.040317	-2.725510
22	6	0	4.118386	-0.006419	-0.979957
23	1	0	5.039401	0.035671	-1.555431
24	6	0	4.165252	-0.060920	0.413916
25	1	0	5.124135	-0.061176	0.925744
26	6	0	2.981194	-0.112786	1.163024
27	1	0	3.036391	-0.153381	2.246747
28	6	0	-1.790837	-1.541528	-1.341924
29	6	0	-1.778659	-1.626679	0.954490
30	8	0	-2.563650	-1.657583	-0.194038
31	8	0	-2.273636	-1.746754	2.040284
32	8	0	-2.284266	-1.558615	-2.434578
33	6	0	0.421494	-0.202216	2.709032
34	1	0	0.979330	-1.082258	3.047841
35	1	0	-0.579998	-0.265202	3.140560
36	1	0	0.918191	0.688816	3.108696

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.516080	0.000000			
3	H	2.189479	1.092888	0.000000		
4	C	1.407384	2.444620	3.398148	0.000000	
5	C	2.447086	1.568384	2.203439	2.859654	0.000000
6	H	2.700328	2.184188	2.508724	3.260017	1.094685
7	C	2.450091	1.517270	2.185283	2.828888	2.486296
8	C	2.831273	2.450158	3.398970	2.460330	2.903372
9	C	2.474584	2.642121	3.734898	1.537659	2.580630
10	C	2.868518	2.545260	3.499204	2.465081	1.542604
11	H	3.290988	3.320532	4.214713	2.729644	2.207804
12	C	3.621894	2.589573	2.753224	4.141398	3.614885
13	H	3.972139	2.837781	2.559645	4.782405	3.936399
14	C	4.143095	3.755268	4.594704	3.646346	4.193973
15	H	4.803712	4.611071	5.535620	4.018840	4.861299
16	C	4.922631	4.297289	4.885398	4.733763	4.947424
17	H	5.962661	5.383527	5.960270	5.677830	5.985349
18	C	4.716543	3.848460	4.142489	4.934754	4.717176
19	H	5.657903	4.740427	4.856578	5.973930	5.644191
20	C	1.392340	2.589680	2.762428	2.433986	3.566646
21	H	2.155103	2.840479	2.572024	3.419416	3.900929
22	C	2.413212	3.848901	4.152337	2.802598	4.659829
23	H	3.398411	4.741846	4.868292	3.889422	5.587353
24	C	2.784395	4.294658	4.891038	2.419758	4.886705
25	H	3.871319	5.380911	5.966499	3.401808	5.923123
26	C	2.420329	3.749482	4.595196	1.394683	4.139355

This journal is © The Royal Society of Chemistry 2014

27	H	3.411898	4.606176	5.535920	2.161577	4.814809
28	C	3.830122	2.566786	2.845559	4.245902	1.519048
29	C	4.249894	3.549536	4.373727	3.866896	2.416049
30	O	4.617637	3.515135	4.042652	4.637167	2.379592
31	O	5.229112	4.659229	5.531380	4.605348	3.596044
32	O	4.537613	3.144592	2.998224	5.201723	2.454099
33	C	3.828403	4.170233	5.262966	2.568316	3.936757
34	H	4.139732	4.669803	5.743296	2.824863	4.230787
35	H	4.642601	4.685443	5.758315	3.514936	4.267564
36	H	4.145251	4.667160	5.734535	2.838822	4.745950

		6	7	8	9	10
6	H	0.000000				
7	C	3.437006	0.000000			
8	C	3.903534	1.407854	0.000000		
9	C	3.339528	2.468206	1.534260	0.000000	
10	C	2.210502	2.879075	2.488789	1.589856	0.000000
11	H	2.386548	3.888065	3.438542	2.190695	1.095241
12	C	4.531004	1.393205	2.433612	3.778659	4.164247
13	H	4.693401	2.155039	3.418728	4.622907	4.808655
14	C	5.237043	2.422890	1.394935	2.614951	3.633357
15	H	5.866467	3.413372	2.160952	2.874282	3.986766
16	C	6.012970	2.785496	2.417795	3.873997	4.718944
17	H	7.061360	3.872334	3.400279	4.763957	5.650831
18	C	5.723073	2.412793	2.799969	4.327786	4.934614
19	H	6.618086	3.397787	3.886709	5.413940	5.968875
20	C	3.483257	3.621440	4.140285	3.784363	4.150714
21	H	3.708803	3.969460	4.779829	4.629450	4.804145
22	C	4.513556	4.718263	4.933788	4.334247	4.914324
23	H	5.330540	5.658967	5.971469	5.420516	5.950266
24	C	4.865202	4.922907	4.731344	3.878236	4.691658
25	H	5.856077	5.961966	5.673134	4.766861	5.622073
26	C	4.337785	4.140554	3.642896	2.616490	3.603763
27	H	5.072198	4.799900	4.013605	2.875434	3.960794
28	C	2.130072	2.975678	3.502144	3.599004	2.425957
29	C	3.164008	3.467669	2.994353	2.612021	1.524899
30	O	3.097174	3.488000	3.520603	3.569308	2.390120
31	O	4.294018	4.381533	3.620932	3.200278	2.464666
32	O	2.786438	3.589383	4.404931	4.699219	3.603162
33	C	4.608745	3.830721	2.575592	1.528187	2.579339
34	H	4.677504	4.634790	3.517577	2.172921	2.811376
35	H	5.033709	4.154544	2.841559	2.176958	2.839128
36	H	5.437906	4.158889	2.857933	2.173046	3.538584

		11	12	13	14	15
11	H	0.000000				
12	C	5.214307	0.000000			
13	H	5.820269	1.087591	0.000000		
14	C	4.548292	2.807854	3.895405	0.000000	
15	H	4.742755	3.893608	4.981140	1.085854	0.000000
16	C	5.726448	2.422566	3.410251	1.401058	2.155594
17	H	6.625536	3.407335	4.308593	2.155694	2.474320
18	C	6.004397	1.400075	2.164296	2.428063	3.407490
19	H	7.048965	2.157674	2.491258	3.412182	4.302596

This journal is © The Royal Society of Chemistry 2014

20	C	4.382784	4.561734	4.681990	5.374777	6.032945
21	H	5.101062	4.675939	4.539849	6.004302	6.776507
22	C	4.926915	5.707893	5.933210	6.065603	6.545551
23	H	5.920160	6.541629	6.649915	7.079253	7.576408
24	C	4.573112	6.047791	6.498757	5.740246	5.997792
25	H	5.391994	7.065132	7.533083	6.579424	6.721759
26	C	3.536139	5.377081	6.010555	4.608236	4.759533
27	H	3.773269	6.033520	6.780712	4.757190	4.657508
28	C	3.166718	3.666464	3.867859	4.501992	5.211057
29	C	2.129121	4.454717	5.134005	3.710479	3.957902
30	O	3.099239	4.173647	4.624667	4.229653	4.721742
31	O	2.787796	5.291488	6.070161	3.984857	3.927260
32	O	4.298257	3.919521	3.804484	5.327676	6.136163
33	C	2.756245	5.006395	5.956552	3.007130	2.673794
34	H	2.539749	5.905152	6.788962	4.092632	3.751245
35	H	3.106115	5.190044	6.183064	2.935945	2.409536
36	H	3.764018	5.208540	6.197925	2.987056	2.487905

		16	17	18	19	20
16	C	0.000000				
17	H	1.086838	0.000000			
18	C	1.396289	2.155791	0.000000		
19	H	2.156855	2.484166	1.086745	0.000000	
20	C	6.042898	7.060846	5.703397	6.538543	0.000000
21	H	6.487212	7.520924	5.921010	6.637540	1.087988
22	C	6.858360	7.804591	6.706414	7.565425	1.401033
23	H	7.797310	8.731134	7.562568	8.355130	2.159202
24	C	6.725378	7.591486	6.860524	7.803089	2.421797
25	H	7.589102	8.390791	7.805521	8.736307	3.407187
26	C	5.741303	6.583517	6.067124	7.083753	2.806161
27	H	5.996850	6.724041	6.545293	7.579079	3.891952
28	C	4.987182	5.943977	4.636541	5.414756	4.928817
29	C	4.650105	5.438570	4.966362	5.914486	5.575649
30	O	4.814363	5.628871	4.791798	5.593863	5.872310
31	O	4.973258	5.576973	5.547861	6.469215	6.569834
32	O	5.556540	6.488786	4.941456	5.532529	5.453931
33	C	4.407828	5.049038	5.236220	6.300796	5.000208
34	H	5.491216	6.143771	6.260250	7.335923	5.172503
35	H	4.278668	4.787942	5.237817	6.257645	5.907780
36	H	4.327766	4.847398	5.272990	6.295857	5.184423

		21	22	23	24	25
21	H	0.000000				
22	C	2.164674	0.000000			
23	H	2.492109	1.086835	0.000000		
24	C	3.409550	1.395725	2.156801	0.000000	
25	H	4.308541	2.155510	2.484509	1.086933	0.000000
26	C	3.894142	2.428351	3.412953	1.402087	2.156655
27	H	4.979940	3.406454	4.301667	2.154564	2.472291
28	C	5.084535	6.116085	7.013222	6.383586	7.426345
29	C	6.135520	6.414239	7.453123	6.170405	7.078148
30	O	6.203265	6.927743	7.907394	6.942411	7.931234
31	O	7.214297	7.280698	8.341865	6.851744	7.668793
32	O	5.374914	6.746791	7.546571	7.207863	8.271547

This journal is © The Royal Society of Chemistry 2014

33	C	5.952957	5.226279	6.290254	4.393546	5.031385
34	H	6.168497	5.218645	6.238914	4.258027	4.767108
35	H	6.796623	6.254634	7.329427	5.476652	6.122432
36	H	6.176427	5.238481	6.258198	4.285715	4.797680

		26	27	28	29	30
26	C	0.000000				
27	H	1.085887	0.000000			
28	C	5.575692	6.173139	0.000000		
29	C	4.999155	5.198581	2.298024	0.000000	
30	O	5.913824	6.291305	1.388651	1.391504	0.000000
31	O	5.572492	5.547779	3.422652	1.199321	2.254830
32	O	6.538977	7.224879	1.199023	3.427251	2.260059
33	C	2.991689	2.655895	4.806081	3.154074	4.411009
34	H	2.915454	2.395009	5.211026	3.504998	4.836681
35	H	4.076269	3.726885	4.815372	2.840653	4.122275
36	H	2.946894	2.437011	5.667564	4.156335	5.341990

		31	32	33	34	35
31	O	0.000000				
32	O	4.478828	0.000000			
33	C	3.177506	5.968055	0.000000		
34	H	3.469655	6.398037	1.095648	0.000000	
35	H	2.504798	5.971567	1.092323	1.762861	0.000000
36	H	4.154667	6.784877	1.095617	1.773173	1.776439

		36
36	H	0.000000

Stoichiometry C19H14O3
Framework group C1[X(C19H14O3)]
Deg. of freedom 102
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.707351	-0.055712	-0.893665
2	6	0	0.299761	-0.051863	-1.456847
3	1	0	0.274301	0.008548	-2.547767
4	6	0	1.747603	-0.115166	0.511887
5	6	0	-0.337137	-1.398487	-0.966141
6	1	0	0.201889	-2.233621	-1.424767
7	6	0	-0.461973	1.078439	-0.790299
8	6	0	-0.425302	1.034090	0.616378
9	6	0	0.364427	-0.153238	1.182536
10	6	0	-0.322381	-1.452233	0.575455
11	1	0	0.212432	-2.327286	0.959918
12	6	0	-1.157996	2.088418	-1.450993
13	1	0	-1.189325	2.108425	-2.537949
14	6	0	-1.091275	2.012206	1.355034
15	1	0	-1.081825	1.988527	2.440588
16	6	0	-1.782479	3.033672	0.690348

This journal is © The Royal Society of Chemistry 2014

17	1	0	-2.297611	3.796640	1.268047
18	6	0	-1.817149	3.072877	-0.704960
19	1	0	-2.358910	3.865323	-1.214412
20	6	0	2.882828	-0.020088	-1.639046
21	1	0	2.840138	0.025501	-2.725240
22	6	0	4.118943	-0.035705	-0.979752
23	1	0	5.040309	-0.000382	-1.555118
24	6	0	4.165282	-0.093385	0.414010
25	1	0	5.124106	-0.102899	0.925860
26	6	0	2.980790	-0.136570	1.162985
27	1	0	3.035592	-0.179798	2.246626
28	6	0	-1.803235	-1.519265	-1.344922
29	6	0	-1.791884	-1.609094	0.951318
30	8	0	-2.577065	-1.630964	-0.197288
31	8	0	-2.287919	-1.727077	2.036859
32	8	0	-2.296748	-1.529933	-2.437619
33	6	0	0.420353	-0.207087	2.708750
34	1	0	0.970593	-1.092563	3.045817
35	1	0	-0.581661	-0.262327	3.140128
36	1	0	0.924670	0.678846	3.110202

Rotational constants (GHZ): 0.4235828 0.2802140 0.2680871

****

Population analysis using the SCF density.

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.23619 -19.17723 -19.17646 -10.35026 -
10.34877
 Alpha  occ. eigenvalues --  -10.24546 -10.24401 -10.24310 -10.23423 -
10.21796
 Alpha  occ. eigenvalues --  -10.21742 -10.21527 -10.21464 -10.21224 -
10.21176
 Alpha  occ. eigenvalues --  -10.21073 -10.21010 -10.20845 -10.20817 -
10.20686
 Alpha  occ. eigenvalues --  -10.20632 -10.19642  -1.15330  -1.08799
-1.04901
 Alpha  occ. eigenvalues --   -0.92439  -0.86974  -0.85180  -0.82344
-0.79413
 Alpha  occ. eigenvalues --   -0.76453  -0.75810  -0.74932  -0.72144
-0.69020
 Alpha  occ. eigenvalues --   -0.67177  -0.64503  -0.61838  -0.61799
-0.60322
 Alpha  occ. eigenvalues --   -0.58041  -0.56369  -0.53864  -0.52793
-0.52100
 Alpha  occ. eigenvalues --   -0.49566  -0.49550  -0.48132  -0.47371
-0.46555
 Alpha  occ. eigenvalues --   -0.45930  -0.45731  -0.45470  -0.44963
-0.44072
 Alpha  occ. eigenvalues --   -0.43568  -0.42930  -0.41811  -0.40828
-0.40134
 Alpha  occ. eigenvalues --   -0.39715  -0.39288  -0.39002  -0.37486
-0.36789
 Alpha  occ. eigenvalues --   -0.35930  -0.35775  -0.34381  -0.34175
-0.34019
 Alpha  occ. eigenvalues --   -0.31645  -0.29201  -0.27114  -0.26962
-0.26586
 Alpha  occ. eigenvalues --   -0.25211
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --   -0.04662  -0.03741  -0.03568  -0.03139
-0.01378
 Alpha virt. eigenvalues --   -0.01264  -0.00657   0.00318   0.00629
0.00730
 Alpha virt. eigenvalues --    0.02282   0.02445   0.03370   0.03571
0.03987
 Alpha virt. eigenvalues --    0.04656   0.04820   0.05476   0.05902
0.06409
 Alpha virt. eigenvalues --    0.06833   0.06895   0.07811   0.08301
0.08410
 Alpha virt. eigenvalues --    0.08860   0.09489   0.10000   0.10227
0.10469
 Alpha virt. eigenvalues --    0.11096   0.11310   0.11995   0.12244
0.12686
 Alpha virt. eigenvalues --    0.12903   0.13199   0.13435   0.13818
0.13961
 Alpha virt. eigenvalues --    0.14139   0.14859   0.15244   0.15569
0.15751
 Alpha virt. eigenvalues --    0.15917   0.16167   0.16467   0.16681
0.17108
 Alpha virt. eigenvalues --    0.17246   0.17601   0.17953   0.18447
0.18830
 Alpha virt. eigenvalues --    0.19149   0.19387   0.19942   0.20231
0.20361
 Alpha virt. eigenvalues --    0.20526   0.20720   0.21095   0.21474
0.21781
 Alpha virt. eigenvalues --    0.21839   0.22272   0.22464   0.22735
0.23121
 Alpha virt. eigenvalues --    0.23434   0.23646   0.24110   0.24346
0.24719
 Alpha virt. eigenvalues --    0.24935   0.25571   0.25596   0.26146
0.26237
 Alpha virt. eigenvalues --    0.26402   0.27096   0.27571   0.27798
0.28055
 Alpha virt. eigenvalues --    0.28365   0.28655   0.28784   0.29589
0.29645
 Alpha virt. eigenvalues --    0.29849   0.30461   0.30970   0.31101
0.31480
 Alpha virt. eigenvalues --    0.32160   0.32492   0.32566   0.33082
0.33198
 Alpha virt. eigenvalues --    0.33911   0.34683   0.34925   0.35153
0.35901
 Alpha virt. eigenvalues --    0.36182   0.36609   0.37322   0.38174
0.38895
 Alpha virt. eigenvalues --    0.39244   0.39549   0.40444   0.41364
0.41526
 Alpha virt. eigenvalues --    0.41921   0.42392   0.42942   0.43351
0.44138
 Alpha virt. eigenvalues --    0.45433   0.46355   0.47345   0.49013
0.51194
 Alpha virt. eigenvalues --    0.52355   0.56193   0.57519   0.58643
0.60147
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.61966   0.64942   0.67262   0.68167
0.68846
 Alpha virt. eigenvalues --    0.69668   0.70805   0.71279   0.71489
0.72040
 Alpha virt. eigenvalues --    0.72537   0.72907   0.73456   0.73900
0.75020
 Alpha virt. eigenvalues --    0.75468   0.76594   0.76789   0.77078
0.77778
 Alpha virt. eigenvalues --    0.78807   0.79055   0.79784   0.80706
0.81211
 Alpha virt. eigenvalues --    0.81650   0.81722   0.82772   0.83417
0.84517
 Alpha virt. eigenvalues --    0.85105   0.85736   0.87183   0.87343
0.88489
 Alpha virt. eigenvalues --    0.89144   0.89259   0.90589   0.91064
0.92440
 Alpha virt. eigenvalues --    0.93814   0.93912   0.94467   0.96038
0.97206
 Alpha virt. eigenvalues --    0.97491   0.99159   0.99785   1.00444
1.00653
 Alpha virt. eigenvalues --    1.02065   1.02662   1.03293   1.04950
1.05338
 Alpha virt. eigenvalues --    1.06007   1.06784   1.08706   1.09691
1.10033
 Alpha virt. eigenvalues --    1.12180   1.14547   1.14793   1.15354
1.16390
 Alpha virt. eigenvalues --    1.17483   1.18395   1.18986   1.19810
1.21936
 Alpha virt. eigenvalues --    1.22355   1.23346   1.24336   1.25688
1.26480
 Alpha virt. eigenvalues --    1.27264   1.28579   1.30378   1.31941
1.32998
 Alpha virt. eigenvalues --    1.33489   1.34895   1.35749   1.36441
1.37091
 Alpha virt. eigenvalues --    1.37165   1.39216   1.39735   1.40344
1.41473
 Alpha virt. eigenvalues --    1.43353   1.43864   1.43950   1.44551
1.45369
 Alpha virt. eigenvalues --    1.46207   1.47078   1.48490   1.48922
1.49511
 Alpha virt. eigenvalues --    1.50330   1.50922   1.53795   1.55328
1.57756
 Alpha virt. eigenvalues --    1.58497   1.61192   1.62885   1.64917
1.68135
 Alpha virt. eigenvalues --    1.70800   1.70943   1.71544   1.73889
1.76631
 Alpha virt. eigenvalues --    1.78201   1.78400   1.78949   1.80927
1.81864
 Alpha virt. eigenvalues --    1.82691   1.83390   1.83655   1.85257
1.86852
 Alpha virt. eigenvalues --    1.87733   1.88289   1.89025   1.89924
1.90616
```

```
 Alpha virt. eigenvalues --    1.91178   1.92564   1.94329   1.95964
1.96783
 Alpha virt. eigenvalues --    1.97401   1.98180   1.98818   2.00773
2.01575
 Alpha virt. eigenvalues --    2.01977   2.02771   2.03872   2.05201
2.07311
 Alpha virt. eigenvalues --    2.07609   2.08729   2.09766   2.12279
2.13390
 Alpha virt. eigenvalues --    2.14350   2.16990   2.17991   2.18446
2.19495
 Alpha virt. eigenvalues --    2.21078   2.22229   2.24032   2.25123
2.26788
 Alpha virt. eigenvalues --    2.28032   2.29261   2.29614   2.31104
2.31766
 Alpha virt. eigenvalues --    2.33687   2.33918   2.36828   2.37432
2.39062
 Alpha virt. eigenvalues --    2.40848   2.43266   2.43920   2.46016
2.49948
 Alpha virt. eigenvalues --    2.51299   2.53261   2.54582   2.58717
2.59833
 Alpha virt. eigenvalues --    2.60702   2.63995   2.65758   2.67009
2.69526
 Alpha virt. eigenvalues --    2.69684   2.71235   2.71825   2.72987
2.75424
 Alpha virt. eigenvalues --    2.76224   2.78397   2.79430   2.80457
2.82907
 Alpha virt. eigenvalues --    2.84087   2.85229   2.85656   2.86456
2.87824
 Alpha virt. eigenvalues --    2.90673   2.94748   2.96558   3.05440
3.09272
 Alpha virt. eigenvalues --    3.11015   3.13358   3.23240   3.23561
3.27099
 Alpha virt. eigenvalues --    3.33850   3.40982   3.41355   4.23957
4.25474
 Alpha virt. eigenvalues --    4.27308   4.31154   4.32708   4.34324
4.36044
 Alpha virt. eigenvalues --    4.39424   4.41505   4.45112   4.48544
4.49043
 Alpha virt. eigenvalues --    4.50890   4.52525   4.60032   4.67475
4.73302
 Alpha virt. eigenvalues --    4.75836   4.80711   4.85107   5.15597
5.37425
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   14.571671  -3.781982  -0.052903   1.908927  -0.120516
0.042228
     2  C   -3.781982  17.246811   0.266121  -4.824703  -1.536018  -
0.051162
     3  H   -0.052903   0.266121   0.532239  -0.010569  -0.001664  -
0.002969
     4  C    1.908927  -4.824703  -0.010569  25.135916   1.593064
0.020713
```

This journal is © The Royal Society of Chemistry 2014

```
     5  C   -0.120516  -1.536018  -0.001664   1.593064  10.882526
0.347673
     6  H    0.042228  -0.051162  -0.002969   0.020713   0.347673
0.481056
     7  C   -0.188030  -4.600453  -0.060238   0.344153   0.624044
0.030517
     8  C    3.895187  -6.754571   0.004225  -0.093671   1.109504
0.016230
     9  C   -2.804621   4.680508  -0.009978  -1.837546  -1.685898  -
0.018019
    10  C    0.397420  -0.472628   0.025802  -0.922934  -2.987348  -
0.021718
    11  H   -0.050366  -0.010483  -0.000125   0.108395  -0.009933  -
0.004619
    12  C   -0.608583   2.136341   0.034531  -0.643102  -0.398009
0.009065
    13  H   -0.020854  -0.025203   0.003326  -0.003789  -0.011912  -
0.000006
    14  C   -2.536167   2.145661   0.000806   0.640239  -0.519789
0.002163
    15  H    0.000976   0.009297   0.000002   0.000278   0.001055
0.000000
    16  C    0.000309  -0.326473   0.003169   0.240518  -0.029843
0.000264
    17  H    0.002453   0.001572   0.000000  -0.003305   0.001053
0.000000
    18  C   -0.293056  -0.039775   0.007024  -0.043186  -0.056805
0.001073
    19  H   -0.003219  -0.016815  -0.000004   0.001823  -0.000431
0.000000
    20  C   -1.133535   0.220572   0.039361  -3.864474   0.527716  -
0.030332
    21  H   -0.021799  -0.046148   0.003376   0.060857   0.010446  -
0.000061
    22  C   -0.747694  -0.466173   0.003067  -0.831018   0.075167  -
0.004891
    23  H    0.007082  -0.014400  -0.000004   0.022265  -0.001209
0.000001
    24  C   -0.254670   0.078014  -0.000227   1.889184  -0.090305
0.005088
    25  H    0.001232   0.001770   0.000000   0.035007   0.000734
0.000000
    26  C    1.340380   0.306168   0.013253 -11.230279  -0.140665  -
0.005302
    27  H    0.032477  -0.001996   0.000003  -0.149254  -0.002572
0.000000
    28  C   -0.571257   0.479331  -0.016915  -0.418399  -1.193119  -
0.081084
    29  C   -0.287826   0.589473  -0.001047  -0.383799   0.494823
0.004501
    30  O   -0.004039   0.130676  -0.000471  -0.005148  -0.345364
0.005418
```

This journal is © The Royal Society of Chemistry 2014

31	O	0.023093	-0.049045	0.000071	-0.009944	-0.027784	-0.000639
32	O	0.003160	-0.076425	0.005058	0.011568	-0.021692	-0.002034
33	C	-2.178514	0.379741	0.004858	-0.837266	-0.185611	0.005183
34	H	-0.012079	0.000399	0.000000	-0.032030	0.008877	-0.000001
35	H	0.006848	-0.010433	0.000000	0.061601	0.002982	0.000002
36	H	-0.029163	0.007372	0.000000	-0.072599	-0.007870	0.000002

		7	8	9	10	11	12
1	C	-0.188030	3.895187	-2.804621	0.397420	-0.050366	-0.608583
2	C	-4.600453	-6.754571	4.680508	-0.472628	-0.010483	2.136341
3	H	-0.060238	0.004225	-0.009978	0.025802	-0.000125	0.034531
4	C	0.344153	-0.093671	-1.837546	-0.922934	0.108395	-0.643102
5	C	0.624044	1.109504	-1.685898	-2.987348	-0.009933	-0.398009
6	H	0.030517	0.016230	-0.018019	-0.021718	-0.004619	0.009065
7	C	18.176283	7.032400	-3.767064	-0.249282	-0.003223	-6.196608
8	C	7.032400	37.496893	-2.991545	-2.315220	-0.014438	-7.711782
9	C	-3.767064	-2.991545	17.802733	-0.402834	-0.045779	1.032185
10	C	-0.249282	-2.315220	-0.402834	11.806991	0.353748	0.331111
11	H	-0.003223	-0.014438	-0.045779	0.353748	0.480088	-0.003116
12	C	-6.196608	-7.711782	1.032185	0.331111	-0.003116	11.622090
13	H	-0.071532	0.047147	0.019566	0.000957	0.000000	0.291427
14	C	-3.991144	-19.514964	0.533287	1.133440	0.023404	5.556974
15	H	0.040115	-0.197597	0.001599	-0.013886	-0.000003	-0.009994
16	C	0.650294	0.259397	-0.055188	-0.008702	0.001424	-1.232519
17	H	0.016286	0.045790	-0.015032	-0.001179	0.000000	0.009784
18	C	-1.758615	-1.045585	0.200107	0.054649	-0.000158	1.346706
19	H	0.017793	0.038441	0.001451	0.000600	0.000000	-0.004721

This journal is © The Royal Society of Chemistry 2014

20	C	1.275794	0.400326	-1.535087	-0.410766	-0.013898	-0.793022
21	H	0.003297	0.004634	0.003488	-0.002866	0.000000	0.001236
22	C	0.084712	0.310888	-0.327578	-0.053010	-0.005372	-0.246186
23	H	-0.003489	0.000578	0.001498	0.000859	0.000000	0.000370
24	C	-0.126412	-0.769466	0.107364	0.338681	0.009248	0.189920
25	H	0.000485	-0.004418	-0.012903	-0.000663	0.000001	-0.000154
26	C	0.602883	2.628227	-0.957440	-0.433496	-0.049457	-0.653219
27	H	0.009115	0.026107	0.015528	0.003110	-0.000072	0.002051
28	C	-0.848299	-0.789101	0.835889	0.563678	0.014562	0.463531
29	C	-0.168308	-0.372741	-0.056348	-0.866357	-0.077408	0.240737
30	O	-0.115603	-0.127472	0.102052	-0.202303	0.005275	0.016095
31	O	0.029683	0.250642	-0.043676	-0.169159	-0.002027	-0.011157
32	O	0.130036	0.048183	-0.042228	-0.068628	-0.000630	-0.093136
33	C	-0.499673	-4.882259	-1.999207	0.622423	0.037299	1.001761
34	H	0.003813	0.036107	-0.053881	-0.070938	0.003478	0.001564
35	H	0.000853	-0.070089	-0.037469	-0.014798	0.000078	0.000863
36	H	0.005783	-0.150544	-0.060926	0.054176	0.000082	0.006521

		13	14	15	16	17	18
1	C	-0.020854	-2.536167	0.000976	0.000309	0.002453	-0.293056
2	C	-0.025203	2.145661	0.009297	-0.326473	0.001572	-0.039775
3	H	0.003326	0.000806	0.000002	0.003169	0.000000	0.007024
4	C	-0.003789	0.640239	0.000278	0.240518	-0.003305	-0.043186
5	C	-0.011912	-0.519789	0.001055	-0.029843	0.001053	-0.056805
6	H	-0.000006	0.002163	0.000000	0.000264	0.000000	0.001073
7	C	-0.071532	-3.991144	0.040115	0.650294	0.016286	-1.758615
8	C	0.047147	-19.514964	-0.197597	0.259397	0.045790	-1.045585

This journal is © The Royal Society of Chemistry 2014

```
     9  C    0.019566   0.533287   0.001599  -0.055188  -0.015032
0.200107
    10  C    0.000957   1.133440  -0.013886  -0.008702  -0.001179
0.054649
    11  H    0.000000   0.023404  -0.000003   0.001424   0.000000  -
0.000158
    12  C    0.291427   5.556974  -0.009994  -1.232519   0.009784
1.346706
    13  H    0.535057  -0.015191   0.000018   0.007433  -0.000161
0.049488
    14  C   -0.015191  21.187750   0.345472  -0.741329   0.013888
0.520309
    15  H    0.000018   0.345472   0.537715   0.076757  -0.004447
0.016537
    16  C    0.007433  -0.741329   0.076757   6.795831   0.286081
0.593032
    17  H   -0.000161   0.013888  -0.004447   0.286081   0.528629  -
0.060081
    18  C    0.049488   0.520309   0.016537   0.593032  -0.060081
6.491042
    19  H   -0.004202  -0.002144  -0.000161  -0.041083  -0.004198
0.304185
    20  C   -0.004238  -0.792131   0.001551   0.019883  -0.000071  -
0.115430
    21  H    0.000000   0.000244   0.000000  -0.000039   0.000000
0.000588
    22  C   -0.000553  -0.241835  -0.000007   0.008077   0.000027  -
0.036912
    23  H    0.000000  -0.000142   0.000000  -0.000009   0.000000  -
0.000005
    24  C   -0.000006   0.432765  -0.001607  -0.034815  -0.000030
0.027600
    25  H    0.000000   0.000739   0.000000   0.000005   0.000000
0.000003
    26  C    0.000015  -2.369558  -0.006185  -0.079904   0.000632  -
0.078135
    27  H    0.000000  -0.006083   0.000000  -0.001563   0.000000
0.000090
    28  C    0.015670   0.702175  -0.000904  -0.025373  -0.001162
0.020925
    29  C   -0.000930   0.105823   0.017327  -0.007857   0.001405
0.028736
    30  O   -0.000110   0.032018  -0.000111  -0.008148  -0.000004
0.006353
    31  O   -0.000001  -0.141798  -0.000737  -0.009191  -0.000033  -
0.005550
    32  O   -0.000211  -0.035931  -0.000002   0.002295   0.000002  -
0.014111
    33  C    0.001982   3.646128   0.000136   0.006437  -0.001930
0.146463
    34  H    0.000000   0.000739   0.000079  -0.001895   0.000000
0.000273
```

This journal is © The Royal Society of Chemistry 2014

35	H	0.000000	0.028185	-0.000763	0.007870	-0.000001	0.000167
36	H	0.000000	0.076561	-0.000681	-0.003586	0.000000	0.001029

		19	20	21	22	23	24
1	C	-0.003219	-1.133535	-0.021799	-0.747694	0.007082	-0.254670
2	C	-0.016815	0.220572	-0.046148	-0.466173	-0.014400	0.078014
3	H	-0.000004	0.039361	0.003376	0.003067	-0.000004	-0.000227
4	C	0.001823	-3.864474	0.060857	-0.831018	0.022265	1.889184
5	C	-0.000431	0.527716	0.010446	0.075167	-0.001209	-0.090305
6	H	0.000000	-0.030332	-0.000061	-0.004891	0.000001	0.005088
7	C	0.017793	1.275794	0.003297	0.084712	-0.003489	-0.126412
8	C	0.038441	0.400326	0.004634	0.310888	0.000578	-0.769466
9	C	0.001451	-1.535087	0.003488	-0.327578	0.001498	0.107364
10	C	0.000600	-0.410766	-0.002866	-0.053010	0.000859	0.338681
11	H	0.000000	-0.013898	0.000000	-0.005372	0.000000	0.009248
12	C	-0.004721	-0.793022	0.001236	-0.246186	0.000370	0.189920
13	H	-0.004202	-0.004238	0.000000	-0.000553	0.000000	-0.000006
14	C	-0.002144	-0.792131	0.000244	-0.241835	-0.000142	0.432765
15	H	-0.000161	0.001551	0.000000	-0.000007	0.000000	-0.001607
16	C	-0.041083	0.019883	-0.000039	0.008077	-0.000009	-0.034815
17	H	-0.004198	-0.000071	0.000000	0.000027	0.000000	-0.000030
18	C	0.304185	-0.115430	0.000588	-0.036912	-0.000005	0.027600
19	H	0.527170	0.000317	0.000000	-0.000004	0.000000	-0.000002
20	C	0.000317	9.706370	0.263693	0.833201	-0.004858	-1.305257
21	H	0.000000	0.263693	0.538349	0.015289	-0.004199	0.012196
22	C	-0.000004	0.833201	0.015289	6.771140	0.307891	0.467643
23	H	0.000000	-0.004858	-0.004199	0.307891	0.527929	-0.028988

24	C	-0.000002	-1.305257	0.012196	0.467643	-0.028988
7.470708						
25	H	0.000000	0.021634	-0.000161	-0.041917	-0.004211
0.302624						
26	C	-0.000219	3.016774	-0.027360	0.641073	0.008313
3.036157						
27	H	0.000000	-0.018130	0.000019	0.023396	-0.000161
0.054439						
28	C	0.001267	-0.266818	0.002431	-0.029070	-0.000016
0.031155						
29	C	-0.001059	0.020211	-0.000557	-0.016636	-0.000063
0.028600						
30	O	-0.000010	0.017460	0.000000	0.002260	0.000000
0.001338						
31	O	0.000004	0.002455	0.000000	0.000267	0.000000
0.002579						
32	O	-0.000030	0.022279	0.000002	0.000392	0.000000
0.000594						
33	C	-0.000009	-0.274530	0.000793	-0.220668	0.000367
0.478219						
34	H	0.000000	-0.002439	0.000000	-0.000806	0.000000
0.014730						
35	H	0.000000	0.001113	0.000000	0.000174	0.000000
0.001900						
36	H	0.000000	-0.001989	0.000000	-0.000688	0.000000
0.010813						

		25	26	27	28	29	30
1	C	0.001232	1.340380	0.032477	-0.571257	-0.287826	
0.004039							
2	C	0.001770	0.306168	-0.001996	0.479331	0.589473	
0.130676							
3	H	0.000000	0.013253	0.000003	-0.016915	-0.001047	
0.000471							
4	C	0.035007	-11.230279	-0.149254	-0.418399	-0.383799	
0.005148							
5	C	0.000734	-0.140665	-0.002572	-1.193119	0.494823	
0.345364							
6	H	0.000000	-0.005302	0.000000	-0.081084	0.004501	
0.005418							
7	C	0.000485	0.602883	0.009115	-0.848299	-0.168308	
0.115603							
8	C	-0.004418	2.628227	0.026107	-0.789101	-0.372741	
0.127472							
9	C	-0.012903	-0.957440	0.015528	0.835889	-0.056348	
0.102052							
10	C	-0.000663	-0.433496	0.003110	0.563678	-0.866357	
0.202303							
11	H	0.000001	-0.049457	-0.000072	0.014562	-0.077408	
0.005275							
12	C	-0.000154	-0.653219	0.002051	0.463531	0.240737	
0.016095							

This journal is © The Royal Society of Chemistry 2014

13	H	0.000000	0.000015	0.000000	0.015670	-0.000930	-0.000110
14	C	0.000739	-2.369558	-0.006083	0.702175	0.105823	0.032018
15	H	0.000000	-0.006185	0.000000	-0.000904	0.017327	-0.000111
16	C	0.000005	-0.079904	-0.001563	-0.025373	-0.007857	-0.008148
17	H	0.000000	0.000632	0.000000	-0.001162	0.001405	-0.000004
18	C	0.000003	-0.078135	0.000090	0.020925	0.028736	0.006353
19	H	0.000000	-0.000219	0.000000	0.001267	-0.001059	-0.000010
20	C	0.021634	3.016774	-0.018130	-0.266818	0.020211	0.017460
21	H	-0.000161	-0.027360	0.000019	0.002431	-0.000557	0.000000
22	C	-0.041917	0.641073	0.023396	-0.029070	-0.016636	0.002260
23	H	-0.004211	0.008313	-0.000161	-0.000016	-0.000063	0.000000
24	C	0.302624	-3.036157	0.054439	0.031155	0.028600	-0.001338
25	H	0.529728	-0.007701	-0.004464	-0.000082	0.000039	0.000000
26	C	-0.007701	18.033970	0.312482	-0.175245	0.030953	0.017386
27	H	-0.004464	0.312482	0.538474	-0.000255	0.002152	-0.000003
28	C	-0.000082	-0.175245	-0.000255	6.621888	-0.755434	0.283347
29	C	0.000039	0.030953	0.002152	-0.755434	6.255759	0.223524
30	O	0.000000	0.017386	-0.000003	0.283347	0.223524	8.360238
31	O	0.000000	0.002186	0.000011	0.026267	0.489171	-0.070004
32	O	0.000000	0.003920	0.000000	0.441997	0.043183	-0.083232
33	C	-0.000309	-1.410365	-0.019370	0.333706	0.143197	-0.002915
34	H	0.000000	0.001588	-0.001028	0.000792	0.001882	-0.000189
35	H	0.000000	-0.011335	0.000078	-0.004904	0.008472	0.000072
36	H	0.000001	-0.012532	-0.000516	0.002337	-0.001266	0.000019

		31	32	33	34	35	36
1	C	0.023093	0.003160	-2.178514	-0.012079	0.006848	-0.029163

This journal is © The Royal Society of Chemistry 2014

```
     2  C   -0.049045  -0.076425   0.379741   0.000399  -0.010433
0.007372
     3  H    0.000071   0.005058   0.004858   0.000000   0.000000
0.000000
     4  C   -0.009944   0.011568  -0.837266  -0.032030   0.061601  -
0.072599
     5  C   -0.027784  -0.021692  -0.185611   0.008877   0.002982  -
0.007870
     6  H   -0.000639  -0.002034   0.005183  -0.000001   0.000002
0.000002
     7  C    0.029683   0.130036  -0.499673   0.003813   0.000853
0.005783
     8  C    0.250642   0.048183  -4.882259   0.036107  -0.070089  -
0.150544
     9  C   -0.043676  -0.042228  -1.999207  -0.053881  -0.037469  -
0.060926
    10  C   -0.169159  -0.068628   0.622423  -0.070938  -0.014798
0.054176
    11  H   -0.002027  -0.000630   0.037299   0.003478   0.000078
0.000082
    12  C   -0.011157  -0.093136   1.001761   0.001564   0.000863
0.006521
    13  H   -0.000001  -0.000211   0.001982   0.000000   0.000000
0.000000
    14  C   -0.141798  -0.035931   3.646128   0.000739   0.028185
0.076561
    15  H   -0.000737  -0.000002   0.000136   0.000079  -0.000763  -
0.000681
    16  C   -0.009191   0.002295   0.006437  -0.001895   0.007870  -
0.003586
    17  H   -0.000033   0.000002  -0.001930   0.000000  -0.000001
0.000000
    18  C   -0.005550  -0.014111   0.146463   0.000273   0.000167
0.001029
    19  H    0.000004  -0.000030  -0.000009   0.000000   0.000000
0.000000
    20  C    0.002455   0.022279  -0.274530  -0.002439   0.001113  -
0.001989
    21  H    0.000000   0.000002   0.000793   0.000000   0.000000
0.000000
    22  C    0.000267   0.000392  -0.220668  -0.000806   0.000174  -
0.000688
    23  H    0.000000   0.000000   0.000367   0.000000   0.000000
0.000000
    24  C   -0.002579  -0.000594   0.478219   0.014730  -0.001900
0.010813
    25  H    0.000000   0.000000  -0.000309   0.000000   0.000000
0.000001
    26  C    0.002186   0.003920  -1.410365   0.001588  -0.011335  -
0.012532
    27  H    0.000011   0.000000  -0.019370  -0.001028   0.000078  -
0.000516
```

This journal is © The Royal Society of Chemistry 2014

```
    28  C    0.026267   0.441997   0.333706   0.000792  -0.004904
0.002337
    29  C    0.489171   0.043183   0.143197   0.001882   0.008472  -
0.001266
    30  O   -0.070004  -0.083232  -0.002915  -0.000189   0.000072
0.000019
    31  O    8.139557   0.000020  -0.038718   0.000707  -0.009904
0.000666
    32  O    0.000020   8.113591  -0.005266  -0.000001   0.000010  -
0.000003
    33  C   -0.038718  -0.005266  10.686588   0.423889   0.374474
0.497903
    34  H    0.000707  -0.000001   0.423889   0.497670  -0.024590  -
0.028269
    35  H   -0.009904   0.000010   0.374474  -0.024590   0.445500  -
0.026433
    36  H    0.000666  -0.000003   0.497903  -0.028269  -0.026433
0.493924
 Mulliken atomic charges:
              1
     1  C   -0.532568
     2  C    0.425058
     3  H    0.210823
     4  C    0.142505
     5  C   -0.305306
     6  H    0.251659
     7  C   -0.430365
     8  C    0.154559
     9  C   -0.577009
    10  C    0.001065
    11  H    0.254028
    12  C    0.310442
    13  H    0.186813
    14  C   -0.220562
    15  H    0.188167
    16  C   -0.351558
    17  H    0.184031
    18  C   -0.268974
    19  H    0.185261
    20  C    0.176294
    21  H    0.182252
    22  C   -0.273649
    23  H    0.184599
    24  C   -0.294637
    25  H    0.182983
    26  C   -0.275649
    27  H    0.185936
    28  C    0.336489
    29  C    0.267668
    30  O   -0.235729
    31  O   -0.372855
    32  O   -0.381543
```

```
    33  C   -0.234935
    34  H    0.231557
    35  H    0.273273
    36  H    0.239874
 Sum of Mulliken atomic charges =   0.00000
 Mulliken charges with hydrogens summed into heavy atoms:
              1
     1  C   -0.532568
     2  C    0.635881
     4  C    0.142505
     5  C   -0.053647
     7  C   -0.430365
     8  C    0.154559
     9  C   -0.577009
    10  C    0.255093
    12  C    0.497255
    14  C   -0.032395
    16  C   -0.167526
    18  C   -0.083713
    20  C    0.358546
    22  C   -0.089049
    24  C   -0.111654
    26  C   -0.089713
    28  C    0.336489
    29  C    0.267668
    30  O   -0.235729
    31  O   -0.372855
    32  O   -0.381543
    33  C    0.509769
 Sum of Mulliken charges with hydrogens summed into heavy atoms =
0.00000
 Electronic spatial extent (au):  <R**2>=           5010.2512
 Charge=              0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=              4.7747    Y=              1.2736    Z=
0.3285  Tot=              4.9526
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=           -135.9038   YY=           -125.1199   ZZ=           -
127.6444
   XY=            -12.4518   XZ=             -1.2484   YZ=
-0.0136
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=             -6.3478   YY=              4.4361   ZZ=
1.9117
   XY=            -12.4518   XZ=             -1.2484   YZ=
-0.0136
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=             58.8117  YYY=            -16.3840  ZZZ=
4.9967  XYY=            -26.8311
  XXY=             27.4140  XXZ=              2.1880  XZZ=
32.8422  YZZ=             23.5963
  YYZ=             -1.5315  XYZ=             -0.5094
```

This journal is © The Royal Society of Chemistry 2014


```
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=          -3304.9404 YYYY=          -1750.6832 ZZZZ=          -
1645.1444 XXXY=            -40.4476
 XXXZ=            -13.8114 YYYX=            -49.8961 YYYZ=
8.4067 ZZZX=            -27.2610
 ZZZY=            -11.8040 XXYY=           -913.5931 XXZZ=           -
868.5044 YYZZ=           -586.9474
 XXYZ=             -5.7926 YYXZ=             11.1708 ZZXY=
-62.5622
 N-N= 1.805868306906D+03 E-N=-5.837012488958D+03  KE=
9.492646206227D+02
 1|1|UNPC-MECHANOCHEM2|FOpt|RB3LYP|6-31+G(d)|C19H14O3|JAMES|25-Jul-
2013
 |0||# opt b3lyp/6-31+g(d) geom=connectivity||9-
methylnanthracene||0,1|
 C,1.7070566202,-0.04697228,-0.8937302687|C,0.2994720635,-
0.0563394888,
 -1.4568614985|H,0.2734678739,0.0016752419,-
2.5478988591|C,1.7478518526
 ,-0.1032761455,0.511935088|C,-0.3258208584,-1.4074047237,-
0.9634457337
 |H,0.2203494364,-2.2387898435,-1.4204283448|C,-
0.4719279755,1.06870360
 78,-0.792536438|C,-
0.434844036,1.0274754349,0.6142247066|C,0.365070263
 7,-0.1518923026,1.1827160609|C,-0.3105668099,-
1.4579482985,0.578254049
 4|H,0.231753597,-2.3276054683,0.9644391319|C,-
1.1766181313,2.071345440
 4,-1.4552139252|H,-1.2081445734,2.0889159243,-2.5422060176|C,-
1.109177
 4371,2.0013052448,1.3509563926|H,-
1.0994984964,1.9798720786,2.43655547
 58|C,-1.8091481824,3.0154676112,0.6842638534|H,-
2.3308013023,3.7751323
 72,1.2604628205|C,-1.8441873633,3.0515914572,-0.7111176722|H,-
2.392748
 3165,3.838335681,-1.2221260504|C,2.8821670047,-0.0027370073,-
1.6392295
 979|H,2.8390606503,0.0403173575,-2.725510358|C,4.1183863537,-
0.0064192
 415,-0.9799569549|H,5.0394008302,0.0356709147,-
1.555430706|C,4.1652522
 928,-0.0609200102,0.4139156097|H,5.1241349997,-
0.0611755852,0.92574379
 81|C,2.9811938422,-0.1127862531,1.1630238557|H,3.0363912739,-
0.1533809
 584,2.2467468057|C,-1.790836836,-1.5415283958,-1.341924233|C,-
1.778658
 579,-1.6266786165,0.9544895181|O,-2.5636502178,-1.6575834937,-
0.194038
```

This journal is © The Royal Society of Chemistry 2014

4199|O,-2.2736355604,-1.7467543499,2.0402844334|O,-2.2842659093,-
1.558
6147181,-2.4345775838|C,0.4214943717,-
0.2022164258,2.7090321164|H,0.97
93296664,-1.0822578549,3.0478406309|H,-0.5799976098,-
0.2652024234,3.14
05604644|H,0.9181912021,0.6888155185,3.1086958503||Version=IA32W-
G09Re
vA.02|State=1-A|HF=-958.1926198|RMSD=9.056e-009|RMSF=1.715e-
005|Dipole
=1.8741554,0.517449,0.1281612|Quadrupole=-
4.5597912,3.1383842,1.421407
,-9.3269548,-0.9093097,-0.0213091|PG=C01 [X(C19H14O3)]||@

FORGIVE MY NONSENSE AS I ALSO FORGIVE THOSE WHO THINK THEY TALK SENSE

-- ROBERT FROST

Job cpu time: 0 days 5 hours 6 minutes 45.0 seconds.
File lengths (MBytes): RWF=   125 Int=   0 D2E=   0 Chk=
13 Scr=   1
Normal termination of Gaussian 09 at Thu Jul 25 04:51:10 2013.

This journal is © The Royal Society of Chemistry 2014

9-formylanthracene-

```
Entering Gaussian System, Link 0=g03
 Initial command:
 /usr/local/g03d01/g03/l1.exe /tmp/pbstmp.6595421/Gau-26905.inp -
scrdir=/tmp/pbstmp.6595421/
 Entering Link 1 = /usr/local/g03d01/g03/l1.exe PID=     26906.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2004, Gaussian, Inc.
                  All Rights Reserved.

 This is the Gaussian(R) 03 program.  It is based on the
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,
 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be
 used, copied, transmitted, or stored only in accord with that
 written license.

 The following legend is applicable only to US Government
 contracts under FAR:

                      RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is
 subject to restrictions as set forth in subparagraphs (a)
 and (c) of the Commercial Computer Software - Restricted
 Rights clause in FAR 52.227-19.

 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ----------------------------------------------------------------
 Warning -- This program may not be used in any manner that
 competes with the business of Gaussian, Inc. or will provide
 assistance to any competitor of Gaussian, Inc.  The licensee
 of this program is prohibited from giving any competitor of
 Gaussian, Inc. access to this program.  By using this program,
 the user acknowledges that Gaussian, Inc. is engaged in the
 business of creating and licensing software in the field of
 computational chemistry and represents and warrants to the
```

This journal is © The Royal Society of Chemistry 2014

```
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.
----------------------------------------------------------------


Cite this work as:
Gaussian 03, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

******************************************
Gaussian 03:  AM64L-G03RevD.01 13-Oct-2005
                2-Nov-2011
******************************************
%nprocshared=1
Will use up to    1 processors via shared memory.
%mem=6MW
%chk=aldehydeanthracene.chk
---------------------------------------
# opt rb3lyp/6-31+g(d) geom=connectivity
---------------------------------------
1/14=-1,18=20,26=3,38=1,57=2/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4/7=1/1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20/3(3);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99//99;
2/9=110/2;
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4/5=5,7=1,16=3/1;
5/5=2,38=5/2;
```

This journal is © The Royal Society of Chemistry 2014

```
 7//1,2,3,16;
 1/14=-1,18=20/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 ------------------
 aldehydeanthracene
 ------------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                    -6.61077  -4.40053   0.01103
 C                    -5.25383  -4.40021   0.01606
 C                    -4.55472  -3.18762   0.01505
 C                    -5.26326  -1.98255   0.00883
 C                    -6.66278  -2.0039    0.0037
 C                    -7.32281  -3.18951   0.00478
 C                    -3.15336  -3.17855   0.02021
 C                    -4.57399  -0.76237   0.00775
 C                    -3.17263  -0.75331   0.01292
 C                    -2.46409  -1.95838   0.01913
 C                    -1.06457  -1.93702   0.02425
 H                    -0.51533  -2.85529   0.02902
 C                    -0.40454  -0.75141   0.02316
 C                    -1.11658   0.45961   0.01691
 C                    -2.47352   0.45929   0.01189
 H                    -2.61104  -4.10092   0.02497
 H                    -7.14199  -5.32935   0.01182
 H                    -4.71845  -5.32663   0.0208
 H                    -7.21202  -1.08563  -0.00107
 H                    -8.39273  -3.20212   0.00085
 H                     0.66538  -0.7388    0.02709
 H                    -0.58536   1.38843   0.01611
 H                    -3.0089    1.38571   0.00714
 C                    -5.35453   0.56515   0.0009
 H                    -6.42449   0.55666  -0.00305
 O                    -4.73399   1.65991  -0.00007



GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Initialization pass.
                            ----------------------------
                            !    Initial Parameters    !
                            ! (Angstroms and Degrees)  !
 --------------------------                             ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ------------------------------------------------------------------------
-----------
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R1    R(1,2)                  1.3569          estimate D2E/DX2
!
 ! R2    R(1,6)                  1.4049          estimate D2E/DX2
!
 ! R3    R(1,17)                 1.07            estimate D2E/DX2
!
 ! R4    R(2,3)                  1.3997          estimate D2E/DX2
!
 ! R5    R(2,18)                 1.07            estimate D2E/DX2
!
 ! R6    R(3,4)                  1.3979          estimate D2E/DX2
!
 ! R7    R(3,7)                  1.4014          estimate D2E/DX2
!
 ! R8    R(4,5)                  1.3997          estimate D2E/DX2
!
 ! R9    R(4,8)                  1.4014          estimate D2E/DX2
!
 ! R10   R(5,6)                  1.3569          estimate D2E/DX2
!
 ! R11   R(5,19)                 1.07            estimate D2E/DX2
!
 ! R12   R(6,20)                 1.07            estimate D2E/DX2
!
 ! R13   R(7,10)                 1.4014          estimate D2E/DX2
!
 ! R14   R(7,16)                 1.07            estimate D2E/DX2
!
 ! R15   R(8,9)                  1.4014          estimate D2E/DX2
!
 ! R16   R(8,24)                 1.54            estimate D2E/DX2
!
 ! R17   R(9,10)                 1.3979          estimate D2E/DX2
!
 ! R18   R(9,15)                 1.3997          estimate D2E/DX2
!
 ! R19   R(10,11)                1.3997          estimate D2E/DX2
!
 ! R20   R(11,12)                1.07            estimate D2E/DX2
!
 ! R21   R(11,13)                1.3569          estimate D2E/DX2
!
 ! R22   R(13,14)                1.4049          estimate D2E/DX2
!
 ! R23   R(13,21)                1.07            estimate D2E/DX2
!
 ! R24   R(14,15)                1.3569          estimate D2E/DX2
!
 ! R25   R(14,22)                1.07            estimate D2E/DX2
!
 ! R26   R(15,23)                1.07            estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R27   R(23,26)              1.7468         estimate D2E/DX2
!
 ! R28   R(24,25)              1.07           estimate D2E/DX2
!
 ! R29   R(24,26)              1.2584         estimate D2E/DX2
!
 ! A1    A(2,1,6)             120.4412        estimate D2E/DX2
!
 ! A2    A(2,1,17)            119.7794        estimate D2E/DX2
!
 ! A3    A(6,1,17)            119.7794        estimate D2E/DX2
!
 ! A4    A(1,2,3)             119.9783        estimate D2E/DX2
!
 ! A5    A(1,2,18)            120.0109        estimate D2E/DX2
!
 ! A6    A(3,2,18)            120.0109        estimate D2E/DX2
!
 ! A7    A(2,3,4)             119.5806        estimate D2E/DX2
!
 ! A8    A(2,3,7)             120.3356        estimate D2E/DX2
!
 ! A9    A(4,3,7)             120.0839        estimate D2E/DX2
!
 ! A10   A(3,4,5)             119.5806        estimate D2E/DX2
!
 ! A11   A(3,4,8)             120.0839        estimate D2E/DX2
!
 ! A12   A(5,4,8)             120.3355        estimate D2E/DX2
!
 ! A13   A(4,5,6)             119.9783        estimate D2E/DX2
!
 ! A14   A(4,5,19)            120.0109        estimate D2E/DX2
!
 ! A15   A(6,5,19)            120.0109        estimate D2E/DX2
!
 ! A16   A(1,6,5)             120.4412        estimate D2E/DX2
!
 ! A17   A(1,6,20)            119.7794        estimate D2E/DX2
!
 ! A18   A(5,6,20)            119.7794        estimate D2E/DX2
!
 ! A19   A(3,7,10)            119.8322        estimate D2E/DX2
!
 ! A20   A(3,7,16)            120.0839        estimate D2E/DX2
!
 ! A21   A(10,7,16)           120.0839        estimate D2E/DX2
!
 ! A22   A(4,8,9)             119.8322        estimate D2E/DX2
!
 ! A23   A(4,8,24)            120.0839        estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A24   A(9,8,24)             120.0839         estimate D2E/DX2
!
 ! A25   A(8,9,10)             120.0839         estimate D2E/DX2
!
 ! A26   A(8,9,15)             120.3356         estimate D2E/DX2
!
 ! A27   A(10,9,15)            119.5806         estimate D2E/DX2
!
 ! A28   A(7,10,9)             120.0839         estimate D2E/DX2
!
 ! A29   A(7,10,11)            120.3355         estimate D2E/DX2
!
 ! A30   A(9,10,11)            119.5806         estimate D2E/DX2
!
 ! A31   A(10,11,12)           120.0109         estimate D2E/DX2
!
 ! A32   A(10,11,13)           119.9783         estimate D2E/DX2
!
 ! A33   A(12,11,13)           120.0109         estimate D2E/DX2
!
 ! A34   A(11,13,14)           120.4412         estimate D2E/DX2
!
 ! A35   A(11,13,21)           119.7794         estimate D2E/DX2
!
 ! A36   A(14,13,21)           119.7794         estimate D2E/DX2
!
 ! A37   A(13,14,15)           120.4412         estimate D2E/DX2
!
 ! A38   A(13,14,22)           119.7794         estimate D2E/DX2
!
 ! A39   A(15,14,22)           119.7794         estimate D2E/DX2
!
 ! A40   A(9,15,14)            119.9783         estimate D2E/DX2
!
 ! A41   A(9,15,23)            120.0109         estimate D2E/DX2
!
 ! A42   A(14,15,23)           120.0109         estimate D2E/DX2
!
 ! A43   A(8,24,25)            120.0            estimate D2E/DX2
!
 ! A44   A(8,24,26)            120.0            estimate D2E/DX2
!
 ! A45   A(25,24,26)           120.0            estimate D2E/DX2
!
 ! D1    D(6,1,2,3)              0.0001         estimate D2E/DX2
!
 ! D2    D(6,1,2,18)          -179.9998         estimate D2E/DX2
!
 ! D3    D(17,1,2,3)          -179.9999         estimate D2E/DX2
!
 ! D4    D(17,1,2,18)            0.0002         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D5    D(2,1,6,5)              0.0           estimate D2E/DX2
!
 ! D6    D(2,1,6,20)          -179.9999        estimate D2E/DX2
!
 ! D7    D(17,1,6,5)          -180.0           estimate D2E/DX2
!
 ! D8    D(17,1,6,20)            0.0           estimate D2E/DX2
!
 ! D9    D(1,2,3,4)             -0.0001        estimate D2E/DX2
!
 ! D10   D(1,2,3,7)           -179.9999        estimate D2E/DX2
!
 ! D11   D(18,2,3,4)           179.9997        estimate D2E/DX2
!
 ! D12   D(18,2,3,7)             0.0           estimate D2E/DX2
!
 ! D13   D(2,3,4,5)              0.0           estimate D2E/DX2
!
 ! D14   D(2,3,4,8)           -179.9997        estimate D2E/DX2
!
 ! D15   D(7,3,4,5)            179.9997        estimate D2E/DX2
!
 ! D16   D(7,3,4,8)              0.0           estimate D2E/DX2
!
 ! D17   D(2,3,7,10)           179.9997        estimate D2E/DX2
!
 ! D18   D(2,3,7,16)             0.0           estimate D2E/DX2
!
 ! D19   D(4,3,7,10)             0.0           estimate D2E/DX2
!
 ! D20   D(4,3,7,16)          -179.9997        estimate D2E/DX2
!
 ! D21   D(3,4,5,6)              0.0001        estimate D2E/DX2
!
 ! D22   D(3,4,5,19)          -180.0           estimate D2E/DX2
!
 ! D23   D(8,4,5,6)            179.9999        estimate D2E/DX2
!
 ! D24   D(8,4,5,19)            -0.0003        estimate D2E/DX2
!
 ! D25   D(3,4,8,9)              0.0           estimate D2E/DX2
!
 ! D26   D(3,4,8,24)           179.9997        estimate D2E/DX2
!
 ! D27   D(5,4,8,9)           -179.9997        estimate D2E/DX2
!
 ! D28   D(5,4,8,24)             0.0           estimate D2E/DX2
!
 ! D29   D(4,5,6,1)              -0.0001        estimate D2E/DX2
!
 ! D30   D(4,5,6,20)           179.9998        estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D31   D(19,5,6,1)           180.0           estimate D2E/DX2
!
 ! D32   D(19,5,6,20)            0.0           estimate D2E/DX2
!
 ! D33   D(3,7,10,9)             0.0           estimate D2E/DX2
!
 ! D34   D(3,7,10,11)         -179.9998         estimate D2E/DX2
!
 ! D35   D(16,7,10,9)          179.9997         estimate D2E/DX2
!
 ! D36   D(16,7,10,11)            0.0           estimate D2E/DX2
!
 ! D37   D(4,8,9,10)              0.0           estimate D2E/DX2
!
 ! D38   D(4,8,9,15)           179.9997         estimate D2E/DX2
!
 ! D39   D(24,8,9,10)         -179.9997         estimate D2E/DX2
!
 ! D40   D(24,8,9,15)             0.0           estimate D2E/DX2
!
 ! D41   D(4,8,24,25)             0.0001        estimate D2E/DX2
!
 ! D42   D(4,8,24,26)         -179.9999         estimate D2E/DX2
!
 ! D43   D(9,8,24,25)          179.9998         estimate D2E/DX2
!
 ! D44   D(9,8,24,26)           -0.0001         estimate D2E/DX2
!
 ! D45   D(8,9,10,7)              0.0           estimate D2E/DX2
!
 ! D46   D(8,9,10,11)          179.9998         estimate D2E/DX2
!
 ! D47   D(15,9,10,7)         -179.9997         estimate D2E/DX2
!
 ! D48   D(15,9,10,11)            0.0           estimate D2E/DX2
!
 ! D49   D(8,9,15,14)         -179.9997         estimate D2E/DX2
!
 ! D50   D(8,9,15,23)             0.0           estimate D2E/DX2
!
 ! D51   D(10,9,15,14)            0.0           estimate D2E/DX2
!
 ! D52   D(10,9,15,23)         179.9997         estimate D2E/DX2
!
 ! D53   D(7,10,11,12)          -0.0001         estimate D2E/DX2
!
 ! D54   D(7,10,11,13)          179.9999         estimate D2E/DX2
!
 ! D55   D(9,10,11,12)         -179.9999         estimate D2E/DX2
!
 ! D56   D(9,10,11,13)            0.0001        estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D57   D(10,11,13,14)         -0.0003         estimate D2E/DX2
!
 ! D58   D(10,11,13,21)        179.9997         estimate D2E/DX2
!
 ! D59   D(12,11,13,14)        179.9998         estimate D2E/DX2
!
 ! D60   D(12,11,13,21)         -0.0002         estimate D2E/DX2
!
 ! D61   D(11,13,14,15)          0.0003         estimate D2E/DX2
!
 ! D62   D(11,13,14,22)       -179.9998         estimate D2E/DX2
!
 ! D63   D(21,13,14,15)       -179.9997         estimate D2E/DX2
!
 ! D64   D(21,13,14,22)          0.0002         estimate D2E/DX2
!
 ! D65   D(13,14,15,9)          -0.0001         estimate D2E/DX2
!
 ! D66   D(13,14,15,23)       -179.9999         estimate D2E/DX2
!
 ! D67   D(22,14,15,9)         179.9999         estimate D2E/DX2
!
 ! D68   D(22,14,15,23)          0.0001         estimate D2E/DX2
!
 ---------------------------------------------------------------------
-----------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
 Number of steps in this run= 152 maximum allowed number of steps=
156.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -6.610774   -4.400532    0.011029
    2          6             0       -5.253834   -4.400213    0.016061
    3          6             0       -4.554722   -3.187617    0.015045
    4          6             0       -5.263261   -1.982548    0.008829
    5          6             0       -6.662784   -2.003900    0.003700
    6          6             0       -7.322813   -3.189510    0.004782
    7          6             0       -3.153361   -3.178550    0.020212
    8          6             0       -4.573989   -0.762374    0.007749
    9          6             0       -3.172628   -0.753307    0.012916
   10          6             0       -2.464089   -1.958375    0.019132
   11          6             0       -1.064566   -1.937024    0.024251
   12          1             0       -0.515332   -2.855294    0.029021
   13          6             0       -0.404537   -0.751414    0.023163
   14          6             0       -1.116576    0.459608    0.016914
```

15	6	0	-2.473516	0.459289	0.011890
16	1	0	-2.611039	-4.100919	0.024966
17	1	0	-7.141991	-5.329352	0.011824
18	1	0	-4.718455	-5.326629	0.020801
19	1	0	-7.212017	-1.085630	-0.001072
20	1	0	-8.392732	-3.202119	0.000852
21	1	0	0.665382	-0.738805	0.027092
22	1	0	-0.585359	1.388428	0.016110
23	1	0	-3.008895	1.385705	0.007142
24	6	0	-5.354527	0.565148	0.000895
25	1	0	-6.424486	0.556658	-0.003048
26	8	0	-4.733986	1.659907	-0.000068

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356949	0.000000			
3	C	2.387159	1.399696	0.000000		
4	C	2.768111	2.417694	1.397947	0.000000	
5	C	2.397207	2.779858	2.417694	1.399696	0.000000
6	C	1.404853	2.397207	2.768111	2.387159	1.356949
7	C	3.667019	2.429911	1.401400	2.425330	3.700828
8	C	4.169495	3.700828	2.425330	1.401400	2.429911
9	C	5.012295	4.198970	2.799295	2.425242	3.707460
10	C	4.812399	3.707460	2.425242	2.799295	4.198970
11	C	6.068729	4.859767	3.707460	4.198970	5.598656
12	H	6.288282	4.984008	4.053061	4.827517	6.206181
13	C	7.199555	6.068729	4.812399	5.012295	6.382379
14	C	7.335339	6.382379	5.012295	4.812399	6.068729
15	C	6.382379	5.598656	4.198970	3.707460	4.859767
16	H	4.010965	2.659703	2.147585	3.394412	4.562300
17	H	1.070000	2.104389	3.358720	3.838063	3.359812
18	H	2.106804	1.070000	2.145277	3.388190	3.849836
19	H	3.369008	3.849836	3.388190	2.145277	1.070000
20	H	2.147480	3.359812	3.838063	3.358720	2.104389
21	H	8.145609	6.960111	5.765961	6.057725	7.436600
22	H	8.355699	7.436600	6.057725	5.765961	6.960111
23	H	6.815723	6.206181	4.827517	4.053061	4.984008
24	C	5.122131	4.966405	3.837073	2.549343	2.882976
25	H	4.960709	5.093266	4.185205	2.792160	2.571631
26	O	6.344397	6.082397	4.850861	3.680719	4.140502

		6	7	8	9	10
6	C	0.000000				
7	C	4.169495	0.000000			
8	C	3.667019	2.802900	0.000000		
9	C	4.812399	2.425330	1.401400	0.000000	
10	C	5.012295	1.401400	2.425330	1.397947	0.000000
11	C	6.382379	2.429911	3.700828	2.417694	1.399696
12	H	6.815723	2.657774	4.566559	3.388190	2.145277
13	C	7.335339	3.667019	4.169495	2.768111	2.387159
14	C	7.199555	4.169495	3.667019	2.387159	2.768111
15	C	6.068729	3.700828	2.429911	1.399696	2.417694

This journal is © The Royal Society of Chemistry 2014

16	H	4.799155	1.070000	3.872900	3.394412	2.147585
17	H	2.147480	4.531577	5.239460	6.057725	5.765961
18	H	3.369008	2.657774	4.566559	4.827517	4.053061
19	H	2.106804	4.566559	2.657774	4.053061	4.827517
20	H	1.070000	5.239460	4.531577	5.765961	6.057725
21	H	8.355699	4.531577	5.239460	3.838063	3.358720
22	H	8.145609	5.239460	4.531577	3.358720	3.838063
23	H	6.288282	4.566559	2.657774	2.145277	3.388190
24	C	4.239295	4.342900	1.540000	2.549343	3.837073
25	H	3.852380	4.965136	2.272510	3.505830	4.691549
26	O	5.497172	5.090133	2.427572	2.874301	4.271389

		11	12	13	14	15
11	C	0.000000				
12	H	1.070000	0.000000			
13	C	1.356949	2.106804	0.000000		
14	C	2.397207	3.369008	1.404853	0.000000	
15	C	2.779858	3.849836	2.397207	1.356949	0.000000
16	H	2.659703	2.437947	4.010965	4.799155	4.562300
17	H	6.960111	7.073462	8.145609	8.355699	7.436600
18	H	4.984008	4.875838	6.288282	6.815723	6.206181
19	H	6.206181	6.926630	6.815723	6.288282	4.984008
20	H	7.436600	7.885081	8.355699	8.145609	6.960111
21	H	2.104389	2.423555	1.070000	2.147480	3.359812
22	H	3.359812	4.244320	2.147480	1.070000	2.104389
23	H	3.849836	4.919798	3.369008	2.106804	1.070000
24	C	4.966405	5.926046	5.122131	4.239295	2.882976
25	H	5.911678	6.823529	6.160481	5.308835	3.952198
26	O	5.138399	6.179395	4.955717	3.811386	2.559561

		16	17	18	19	20
16	H	0.000000				
17	H	4.694544	0.000000			
18	H	2.437947	2.423555	0.000000		
19	H	5.501059	4.244320	4.919798	0.000000	
20	H	5.851187	2.467710	4.244320	2.423555	0.000000
21	H	4.694544	9.056955	7.073462	7.885081	9.387120
22	H	5.851187	9.387120	7.885081	7.073462	9.056955
23	H	5.501059	7.885081	6.926630	4.875838	7.073462
24	C	5.412900	6.159568	5.926046	2.485023	4.839730
25	H	6.019650	5.929600	6.125698	1.821351	4.242925
26	O	6.139597	7.392454	6.986585	3.698461	6.084876

		21	22	23	24	25
21	H	0.000000				
22	H	2.467710	0.000000			
23	H	4.244320	2.423555	0.000000		
24	C	6.159568	4.839730	2.485023	0.000000	
25	H	7.207313	5.898103	3.514781	1.070000	0.000000
26	O	5.908276	4.157531	1.746762	1.258400	2.018653

		26
26	O	0.000000

Stoichiometry C15H10O
Framework group C1[X(C15H10O)]
Deg. of freedom 72

This journal is © The Royal Society of Chemistry 2014

```
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6              0        3.746198   -0.864754    0.000005
    2          6              0        2.630395   -1.636955    0.000002
    3          6              0        1.365333   -1.037984   -0.000004
    4          6              0        1.261871    0.356129   -0.000005
    5          6              0        2.424657    1.135279    0.000000
    6          6              0        3.642225    0.536246    0.000003
    7          6              0        0.208028   -1.828280   -0.000004
    8          6              0        0.000585    0.966933   -0.000005
    9          6              0       -1.156720    0.176637   -0.000005
   10          6              0       -1.053258   -1.217476   -0.000004
   11          6              0       -2.216044   -1.996626    0.000001
   12          1              0       -2.144870   -3.064256    0.000003
   13          6              0       -3.433612   -1.397593    0.000003
   14          6              0       -3.537585    0.003407    0.000005
   15          6              0       -2.421782    0.775608    0.000000
   16          1              0        0.287219   -2.895345    0.000000
   17          1              0        4.711682   -1.325992    0.000007
   18          1              0        2.717597   -2.703396    0.000006
   19          1              0        2.353483    2.202910    0.000000
   20          1              0        4.529047    1.134950    0.000005
   21          1              0       -4.320434   -1.996297    0.000003
   22          1              0       -4.503069    0.464645    0.000011
   23          1              0       -2.508984    1.842049    0.000003
   24          6              0       -0.113390    2.502709    0.000000
   25          1              0        0.771120    3.104823    0.000002
   26          8              0       -1.246775    3.049527    0.000001
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      1.0171063      0.4571266
0.3153819
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   324 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   324 basis functions,   552 primitive gaussians,   324 cartesian
basis functions
    54 alpha electrons       54 beta electrons
       nuclear repulsion energy       980.1292881223 Hartrees.
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   324 RedAO= T  NBF=   324
 NBsUse=   317 1.00D-06 NBFU=   317
 Harris functional with IExCor=  402 diagonalized for initial guess.
```

```
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Restarting incremental Fock formation.
 SCF Done:  E(RB+HF-LYP) =  -652.841781469     A.U. after   22 cycles
             Convg  =    0.2082D-08             -V/T =  2.0080
             S**2   =   0.0000


**********************************************************************

           Population analysis using the SCF density.


**********************************************************************

 Orbital symmetries:
```

```
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.15424 -10.28842 -10.21602 -10.21553 -
10.21339
 Alpha  occ. eigenvalues --  -10.21183 -10.20860 -10.20677 -10.20518 -
10.20377
 Alpha  occ. eigenvalues --  -10.20240 -10.20217 -10.19699 -10.19533 -
10.19203
 Alpha  occ. eigenvalues --  -10.17430  -1.03361  -0.91134  -0.87638
-0.82298
 Alpha  occ. eigenvalues --   -0.81068  -0.77176  -0.76082  -0.72498
-0.67291
 Alpha  occ. eigenvalues --   -0.65432  -0.63439  -0.61018  -0.59453
-0.55421
 Alpha  occ. eigenvalues --   -0.54488  -0.52037  -0.48261  -0.48018
-0.47746
 Alpha  occ. eigenvalues --   -0.47155  -0.45895  -0.43623  -0.43111
-0.42331
 Alpha  occ. eigenvalues --   -0.41772  -0.40580  -0.39038  -0.38775
-0.38116
 Alpha  occ. eigenvalues --   -0.36556  -0.35942  -0.34406  -0.31954
-0.31236
 Alpha  occ. eigenvalues --   -0.27179  -0.26039  -0.25105  -0.21254
 Alpha virt. eigenvalues --   -0.09811  -0.04359  -0.02490  -0.00712
-0.00002
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.00704   0.01337   0.02155   0.02589
0.03129
 Alpha virt. eigenvalues --    0.03992   0.04677   0.05171   0.05277
0.05421
 Alpha virt. eigenvalues --    0.06742   0.07270   0.07330   0.07375
0.07572
 Alpha virt. eigenvalues --    0.09205   0.09638   0.09731   0.10893
0.11805
 Alpha virt. eigenvalues --    0.11857   0.12151   0.12976   0.13476
0.13902
 Alpha virt. eigenvalues --    0.14108   0.14337   0.15188   0.15829
0.16872
 Alpha virt. eigenvalues --    0.17530   0.17567   0.17845   0.18151
0.18683
 Alpha virt. eigenvalues --    0.18947   0.19032   0.19427   0.19572
0.20390
 Alpha virt. eigenvalues --    0.20490   0.20666   0.21472   0.22233
0.22611
 Alpha virt. eigenvalues --    0.23163   0.23799   0.23878   0.24495
0.24908
 Alpha virt. eigenvalues --    0.25148   0.25194   0.25480   0.26487
0.26955
 Alpha virt. eigenvalues --    0.27514   0.28041   0.28258   0.29029
0.29571
 Alpha virt. eigenvalues --    0.29852   0.30510   0.31007   0.31117
0.31556
 Alpha virt. eigenvalues --    0.31810   0.32645   0.32892   0.34292
0.34957
 Alpha virt. eigenvalues --    0.35802   0.36100   0.37334   0.38714
0.39199
 Alpha virt. eigenvalues --    0.39994   0.40593   0.42815   0.43948
0.45554
 Alpha virt. eigenvalues --    0.46136   0.49719   0.50378   0.53502
0.59900
 Alpha virt. eigenvalues --    0.60734   0.63483   0.64309   0.66103
0.66291
 Alpha virt. eigenvalues --    0.66628   0.67044   0.67253   0.69958
0.71059
 Alpha virt. eigenvalues --    0.71533   0.72201   0.72357   0.72608
0.73710
 Alpha virt. eigenvalues --    0.74079   0.74188   0.74473   0.75968
0.76158
 Alpha virt. eigenvalues --    0.76968   0.77968   0.78025   0.79218
0.79820
 Alpha virt. eigenvalues --    0.80115   0.80117   0.82481   0.82589
0.86078
 Alpha virt. eigenvalues --    0.88419   0.90270   0.91184   0.91279
0.91798
 Alpha virt. eigenvalues --    0.92357   0.93400   0.95714   0.96552
0.98005
 Alpha virt. eigenvalues --    1.00645   1.02264   1.04154   1.06072
1.07547
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    1.09042   1.10555   1.11894   1.12320
1.14876
 Alpha virt. eigenvalues --    1.17756   1.18668   1.19313   1.19652
1.20606
 Alpha virt. eigenvalues --    1.20788   1.22045   1.22136   1.23046
1.24565
 Alpha virt. eigenvalues --    1.25841   1.26927   1.28386   1.31591
1.31636
 Alpha virt. eigenvalues --    1.33505   1.34746   1.36329   1.38524
1.38535
 Alpha virt. eigenvalues --    1.42684   1.42809   1.44978   1.45695
1.47304
 Alpha virt. eigenvalues --    1.47964   1.48209   1.48338   1.48519
1.49870
 Alpha virt. eigenvalues --    1.51212   1.53910   1.56142   1.56476
1.58650
 Alpha virt. eigenvalues --    1.63780   1.72315   1.73015   1.74476
1.78477
 Alpha virt. eigenvalues --    1.79968   1.83638   1.84522   1.84782
1.87171
 Alpha virt. eigenvalues --    1.89629   1.92292   1.94296   1.95127
1.95858
 Alpha virt. eigenvalues --    1.97747   1.98564   1.99171   2.00304
2.00961
 Alpha virt. eigenvalues --    2.02817   2.06659   2.07551   2.08025
2.08554
 Alpha virt. eigenvalues --    2.11397   2.12568   2.18384   2.20031
2.20227
 Alpha virt. eigenvalues --    2.22472   2.24015   2.25196   2.28629
2.29750
 Alpha virt. eigenvalues --    2.29828   2.30221   2.32347   2.33096
2.36490
 Alpha virt. eigenvalues --    2.38844   2.40278   2.42350   2.44164
2.48075
 Alpha virt. eigenvalues --    2.52698   2.55182   2.57779   2.59600
2.62759
 Alpha virt. eigenvalues --    2.67699   2.69308   2.70606   2.70805
2.73951
 Alpha virt. eigenvalues --    2.74644   2.76634   2.77480   2.80490
2.84088
 Alpha virt. eigenvalues --    2.87177   2.87631   2.91594   2.97677
2.99312
 Alpha virt. eigenvalues --    3.01970   3.09871   3.14503   3.20273
3.38279
 Alpha virt. eigenvalues --    3.53604   3.54324   4.20800   4.24298
4.26321
 Alpha virt. eigenvalues --    4.26789   4.29475   4.31146   4.32743
4.34381
 Alpha virt. eigenvalues --    4.35576   4.41514   4.41765   4.43756
4.49722
 Alpha virt. eigenvalues --    4.52684   4.69549   4.90911
          Condensed to atoms (all electrons):
```

This journal is © The Royal Society of Chemistry 2014

		1	2	3	4	5	6
1	C	6.182546	0.228870	-0.626709	0.883646	-1.166966	1.201803
2	C	0.228870	7.994444	-0.452896	-0.442922	1.869257	-1.534969
3	C	-0.626709	-0.452896	8.726494	-0.968588	1.428100	-0.298162
4	C	0.883646	-0.442922	-0.968588	11.210287	-3.716887	1.139122
5	C	-1.166966	1.869257	1.428100	-3.716887	12.141964	-2.852664
6	C	1.201803	-1.534969	-0.298162	1.139122	-2.852664	8.262169
7	C	-0.353552	-0.667155	1.218649	-1.907862	0.876890	-0.299914
8	C	0.079405	-0.441263	-0.357023	1.277106	-1.658962	0.472401
9	C	-0.055871	-0.436613	-1.455857	0.074185	-0.515867	0.232530
10	C	-0.195250	-0.133818	-1.162286	-1.388914	0.133172	-0.210887
11	C	-0.014788	-0.107200	0.181292	-0.324536	-0.234368	-0.019246
12	H	0.000369	0.001958	-0.018279	0.000578	0.000479	-0.000044
13	C	0.010110	-0.081418	-0.222374	-0.046479	-0.016163	0.002117
14	C	-0.013095	-0.037514	-0.120962	0.438551	0.205229	0.001089
15	C	-0.010979	0.027924	0.250398	-0.528005	-0.426161	0.077044
16	H	-0.007864	-0.019044	-0.063412	0.000461	0.003009	0.001253
17	H	0.310527	-0.010278	-0.004705	0.021448	0.011902	-0.018569
18	H	0.024016	0.264307	-0.047089	0.071122	-0.042025	0.016079
19	H	0.011727	-0.034671	-0.001076	-0.013814	0.234470	0.020920
20	H	-0.020413	0.017732	0.022376	-0.039793	0.030750	0.291289
21	H	0.000020	0.000228	-0.002142	-0.000352	-0.000089	-0.000010
22	H	0.000003	-0.000079	0.000406	-0.002226	0.000076	0.000028
23	H	-0.000257	-0.000311	0.000660	0.014211	0.001373	0.000320
24	C	0.007481	0.149678	-0.248089	-0.024453	0.183426	-0.158054
25	H	0.001133	0.002851	-0.037169	0.022643	-0.011050	0.008690

This journal is © The Royal Society of Chemistry 2014

26	O	0.001283	-0.006153	-0.004493	-0.009873	0.024721	0.014023

		7	8	9	10	11	12
1	C	-0.353552	0.079405	-0.055871	-0.195250	-0.014788	0.000369
2	C	-0.667155	-0.441263	-0.436613	-0.133818	-0.107200	0.001958
3	C	1.218649	-0.357023	-1.455857	-1.162286	0.181292	-0.018279
4	C	-1.907862	1.277106	0.074185	-1.388914	-0.324536	0.000578
5	C	0.876890	-1.658962	-0.515867	0.133172	-0.234368	0.000479
6	C	-0.299914	0.472401	0.232530	-0.210887	-0.019246	-0.000044
7	C	8.206980	-0.467922	-1.678526	0.554769	0.010233	-0.023008
8	C	-0.467922	7.345473	1.266616	-0.130429	-0.264437	0.006079
9	C	-1.678526	1.266616	11.683870	-0.008034	-1.222086	0.074052
10	C	0.554769	-0.130429	-0.008034	8.892359	-0.579453	-0.038425
11	C	0.010233	-0.264437	-1.222086	-0.579453	7.835783	0.265445
12	H	-0.023008	0.006079	0.074052	-0.038425	0.265445	0.546175
13	C	-0.331122	-0.007250	1.027327	-0.598170	0.228799	0.030045
14	C	-0.529379	0.365830	0.844412	0.214647	-1.859184	0.019645
15	C	1.089298	-1.097290	-3.972967	0.810561	2.185648	-0.043474
16	H	0.346542	0.002516	0.020192	-0.023336	0.004974	0.004120
17	H	-0.012748	-0.000374	0.000342	-0.002835	0.000014	0.000000
18	H	-0.013740	0.009214	0.000442	-0.013551	0.005902	0.000002
19	H	0.001770	0.039655	0.013845	0.000877	0.000144	0.000000
20	H	0.005029	-0.009758	-0.002369	0.001199	-0.000037	0.000000
21	H	-0.010075	0.002412	0.030876	-0.016518	-0.009159	-0.005253
22	H	0.003258	-0.007854	-0.016362	0.007194	0.014220	-0.000197
23	H	-0.002204	-0.007588	-0.129313	0.044231	-0.019248	0.000020
24	C	-0.047754	-0.505814	-0.378931	-0.322118	0.021869	-0.000037

This journal is © The Royal Society of Chemistry 2014

25	H	-0.001617	-0.165261	-0.012566	-0.011151	-0.003351	0.000000
26	O	0.024044	0.028539	-0.097166	0.026399	-0.028990	-0.000004

		13	14	15	16	17	18
1	C	0.010110	-0.013095	-0.010979	-0.007864	0.310527	0.024016
2	C	-0.081418	-0.037514	0.027924	-0.019044	-0.010278	0.264307
3	C	-0.222374	-0.120962	0.250398	-0.063412	-0.004705	-0.047089
4	C	-0.046479	0.438551	-0.528005	0.000461	0.021448	0.071122
5	C	-0.016163	0.205229	-0.426161	0.003009	0.011902	-0.042025
6	C	0.002117	0.001089	0.077044	0.001253	-0.018569	0.016079
7	C	-0.331122	-0.529379	1.089298	0.346542	-0.012748	-0.013740
8	C	-0.007250	0.365830	-1.097290	0.002516	-0.000374	0.009214
9	C	1.027327	0.844412	-3.972967	0.020192	0.000342	0.000442
10	C	-0.598170	0.214647	0.810561	-0.023336	-0.002835	-0.013551
11	C	0.228799	-1.859184	2.185648	0.004974	0.000014	0.005902
12	H	0.030045	0.019645	-0.043474	0.004120	0.000000	0.000002
13	C	6.308990	1.159000	-1.231922	0.000862	-0.000004	0.000787
14	C	1.159000	9.251766	-3.615280	0.003537	0.000001	-0.000136
15	C	-1.231922	-3.615280	12.630033	0.002487	-0.000020	0.000255
16	H	0.000862	0.003537	0.002487	0.527937	-0.000015	0.004164
17	H	-0.000004	0.000001	-0.000020	-0.000015	0.534841	-0.005160
18	H	0.000787	-0.000136	0.000255	0.004164	-0.005160	0.542497
19	H	0.000036	-0.000590	-0.001371	0.000002	-0.000210	0.000023
20	H	0.000003	0.000015	-0.000069	0.000000	-0.004449	-0.000194
21	H	0.301997	-0.048613	0.043901	-0.000016	0.000000	0.000000
22	H	-0.037419	0.319575	0.013649	0.000000	0.000000	0.000000
23	H	0.015856	0.089766	0.343388	0.000002	0.000000	0.000000

This journal is © The Royal Society of Chemistry 2014

24	C	-0.053202	-0.180996	0.058510	0.001541	0.000400	-0.000139
25	H	-0.000374	0.002957	0.003495	0.000000	0.000000	0.000000
26	O	-0.022505	0.019375	-0.081241	-0.000004	0.000000	0.000000

		19	20	21	22	23	24
1	C	0.011727	-0.020413	0.000020	0.000003	-0.000257	0.007481
2	C	-0.034671	0.017732	0.000228	-0.000079	-0.000311	0.149678
3	C	-0.001076	0.022376	-0.002142	0.000406	0.000660	-0.248089
4	C	-0.013814	-0.039793	-0.000352	-0.002226	0.014211	-0.024453
5	C	0.234470	0.030750	-0.000089	0.000076	0.001373	0.183426
6	C	0.020920	0.291289	-0.000010	0.000028	0.000320	-0.158054
7	C	0.001770	0.005029	-0.010075	0.003258	-0.002204	-0.047754
8	C	0.039655	-0.009758	0.002412	-0.007854	-0.007588	-0.505814
9	C	0.013845	-0.002369	0.030876	-0.016362	-0.129313	-0.378931
10	C	0.000877	0.001199	-0.016518	0.007194	0.044231	-0.322118
11	C	0.000144	-0.000037	-0.009159	0.014220	-0.019248	0.021869
12	H	0.000000	0.000000	-0.005253	-0.000197	0.000020	-0.000037
13	C	0.000036	0.000003	0.301997	-0.037419	0.015856	-0.053202
14	C	-0.000590	0.000015	-0.048613	0.319575	0.089766	-0.180996
15	C	-0.001371	-0.000069	0.043901	0.013649	0.343388	0.058510
16	H	0.000002	0.000000	-0.000016	0.000000	0.000002	0.001541
17	H	-0.000210	-0.004449	0.000000	0.000000	0.000000	0.000400
18	H	0.000023	-0.000194	0.000000	0.000000	0.000000	-0.000139
19	H	0.567706	-0.005258	0.000000	0.000000	-0.000004	-0.007702
20	H	-0.005258	0.534152	0.000000	0.000000	0.000000	-0.001228
21	H	0.000000	0.000000	0.539232	-0.004185	-0.000195	0.000721
22	H	0.000000	0.000000	-0.004185	0.535422	-0.005383	-0.001527

This journal is © The Royal Society of Chemistry 2014

```
    23  H   -0.000004   0.000000  -0.000195  -0.005383   0.463088  -
0.050179
    24  C   -0.007702  -0.001228   0.000721  -0.001527  -0.050179
6.867366
    25  H    0.003540   0.000018   0.000000   0.000000  -0.000261
0.489479
    26  O    0.002192   0.000001   0.000037   0.000747  -0.032271
0.281352
              25         26
     1  C    0.001133   0.001283
     2  C    0.002851  -0.006153
     3  C   -0.037169  -0.004493
     4  C    0.022643  -0.009873
     5  C   -0.011050   0.024721
     6  C    0.008690   0.014023
     7  C   -0.001617   0.024044
     8  C   -0.165261   0.028539
     9  C   -0.012566  -0.097166
    10  C   -0.011151   0.026399
    11  C   -0.003351  -0.028990
    12  H    0.000000  -0.000004
    13  C   -0.000374  -0.022505
    14  C    0.002957   0.019375
    15  C    0.003495  -0.081241
    16  H    0.000000  -0.000004
    17  H    0.000000   0.000000
    18  H    0.000000   0.000000
    19  H    0.003540   0.002192
    20  H    0.000018   0.000001
    21  H    0.000000   0.000037
    22  H    0.000000   0.000747
    23  H   -0.000261  -0.032271
    24  C    0.489479   0.281352
    25  H    0.600508  -0.064140
    26  O   -0.064140   8.307680
 Mulliken atomic charges:
              1
     1  C   -0.477194
     2  C   -0.150945
     3  C    0.262937
     4  C    0.261344
     5  C   -0.503617
     6  C   -0.348360
     7  C    0.009115
     8  C    0.225979
     9  C    0.713839
    10  C    0.149767
    11  C   -0.068241
    12  H    0.179753
    13  C   -0.437527
    14  C   -0.529643
    15  C   -0.527811
```

This journal is © The Royal Society of Chemistry 2014

```
   16  H    0.190091
   17  H    0.179892
   18  H    0.183222
   19  H    0.167790
   20  H    0.181003
   21  H    0.177183
   22  H    0.180654
   23  H    0.274298
   24  C   -0.081600
   25  H    0.171627
   26  O   -0.383554
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  C   -0.297302
    2  C    0.032277
    3  C    0.262937
    4  C    0.261344
    5  C   -0.335827
    6  C   -0.167357
    7  C    0.199205
    8  C    0.225979
    9  C    0.713839
   10  C    0.149767
   11  C    0.111513
   12  H    0.000000
   13  C   -0.260344
   14  C   -0.348989
   15  C   -0.253513
   16  H    0.000000
   17  H    0.000000
   18  H    0.000000
   19  H    0.000000
   20  H    0.000000
   21  H    0.000000
   22  H    0.000000
   23  H    0.000000
   24  C    0.090027
   25  H    0.000000
   26  O   -0.383554
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  3339.1111
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     2.1901    Y=    -2.6578    Z=     0.0000  Tot=     3.4439
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -81.6381   YY=   -90.6567   ZZ=   -97.6262
  XY=     7.2600   XZ=     0.0000   YZ=     0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     8.3355   YY=    -0.6830   ZZ=    -7.6525
  XY=     7.2600   XZ=     0.0000   YZ=     0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
```

This journal is © The Royal Society of Chemistry 2014

```
  XXX=     1.1643  YYY=   -37.9062  ZZZ=     0.0000  XYY=    26.1942
  XXY=    -6.2612  XXZ=     0.0002  XZZ=    -2.6026  YZZ=     8.0903
  YYZ=     0.0001  XYZ=     0.0000
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX= -2801.1479 YYYY= -1449.8080 ZZZZ=  -115.9454 XXXY=     2.7053
 XXXZ=     0.0000 YYYX=    78.7164 YYYZ=    -0.0003 ZZZX=     0.0000
 ZZZY=     0.0000 XXYY=  -723.1446 XXZZ=  -602.1325 YYZZ=  -267.9104
 XXYZ=    -0.0001 YYXZ=     0.0001 ZZXY=    -7.6432
 N-N= 9.801292881223D+02 E-N=-3.474740366142D+03  KE=
6.476444959398D+02
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.004335945   -0.008232977    0.000008479
    2          6          -0.008037484   -0.009250745   -0.000002265
    3          6           0.030277208   -0.017897847    0.000165412
    4          6          -0.005357569    0.029198055   -0.000106992
    5          6          -0.012594300   -0.004070001   -0.000034376
    6          6          -0.007297302   -0.000788927   -0.000024611
    7          6          -0.010420473    0.018273426   -0.000093032
    8          6          -0.025934261    0.033275403   -0.000195383
    9          6          -0.020683730    0.020509980   -0.000137798
   10          6          -0.000046605   -0.035246137    0.000104611
   11          6           0.011735630    0.000897935    0.000041050
   12          1           0.004922270   -0.011867547    0.000053698
   13          6           0.010108785    0.001500111    0.000032930
   14          6           0.006924046   -0.001570628    0.000030557
   15          6           0.018083918    0.014178661    0.000024554
   16          1           0.006111954   -0.010703164    0.000054591
   17          1          -0.006982006   -0.010447239    0.000005136
   18          1           0.007795939   -0.010043085    0.000058937
   19          1          -0.006901984    0.004284351   -0.000038343
   20          1          -0.012586116   -0.000947746   -0.000043927
   21          1           0.012996167    0.000367943    0.000046893
   22          1           0.006778609    0.010687553   -0.000006729
   23          1           0.004483714   -0.000157881    0.000017212
   24          6           0.075457987    0.012228707    0.000243565
   25          1          -0.017563793    0.000916892   -0.000067898
   26          8          -0.056934659   -0.025095095   -0.000136269
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.075457987 RMS     0.015588501


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.040841483 RMS     0.010894422
 Search for a local minimum.
 Step number   1 out of a maximum of 152
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
```

This journal is © The Royal Society of Chemistry 2014

```
 Second derivative matrix not updated -- first step.
     Eigenvalues ---    0.00237   0.00237   0.01518   0.02070
0.02070
     Eigenvalues ---    0.02084   0.02085   0.02088   0.02088
0.02093
     Eigenvalues ---    0.02097   0.02227   0.02229   0.02251
0.02256
     Eigenvalues ---    0.02348   0.02348   0.02376   0.02376
0.02422
     Eigenvalues ---    0.02426   0.02499   0.02502   0.07507
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16510
0.22000
     Eigenvalues ---    0.22000   0.22418   0.22553   0.22718
0.23589
     Eigenvalues ---    0.24495   0.24609   0.25000   0.25000
0.28426
     Eigenvalues ---    0.36503   0.37230   0.37230   0.37230
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37230   0.37230
0.37230
     Eigenvalues ---    0.37743   0.40428   0.41485   0.42818
0.42954
     Eigenvalues ---    0.43653   0.45037   0.45286   0.45324
0.45389
     Eigenvalues ---    0.45602   0.45785   0.51533   0.51546
0.52879
     Eigenvalues ---    0.52922
0.799461000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-4.20528174D-02.
 Linear search not attempted -- first point.
 Maximum step size (   0.300) exceeded in Quadratic search.
    -- Step size scaled by   0.806
 Iteration  1 RMS(Cart)=  0.04996988 RMS(Int)=  0.00058294
 Iteration  2 RMS(Cart)=  0.00073405 RMS(Int)=  0.00005417
 Iteration  3 RMS(Cart)=  0.00000050 RMS(Int)=  0.00005417
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.56426   0.01714   0.00000   0.02284   0.02272
2.58699
    R2        2.65479   0.01579   0.00000   0.02428   0.02415
2.67894
    R3        2.02201   0.01253   0.00000   0.02439   0.02439
2.04640
    R4        2.64504   0.02866   0.00000   0.04675   0.04677
2.69181
    R5        2.02201   0.01259   0.00000   0.02451   0.02451
2.04652
    R6        2.64174   0.03901   0.00000   0.06363   0.06379
2.70553
    R7        2.64826   0.00472   0.00000   0.00430   0.00428
2.65254
    R8        2.64504   0.03382   0.00000   0.05591   0.05602
2.70106
    R9        2.64826   0.02977   0.00000   0.05105   0.05109
2.69936
   R10        2.56426   0.02138   0.00000   0.02946   0.02944
2.59371
   R11        2.02201   0.00722   0.00000   0.01406   0.01406
2.03606
   R12        2.02201   0.01260   0.00000   0.02452   0.02452
2.04652
   R13        2.64826   0.00309   0.00000   0.00239   0.00234
2.65061
   R14        2.02201   0.01232   0.00000   0.02399   0.02399
2.04599
   R15        2.64826   0.02081   0.00000   0.04174   0.04177
2.69003
   R16        2.91018  -0.02723   0.00000  -0.06268  -0.06268
2.84750
   R17        2.64174   0.03429   0.00000   0.05795   0.05797
2.69971
```

This journal is © The Royal Society of Chemistry 2014

R18	2.64504	0.02206	0.00000	0.03921	0.03926
2.68430					
R19	2.64504	0.02850	0.00000	0.04625	0.04625
2.69129					
R20	2.02201	0.01271	0.00000	0.02474	0.02474
2.04675					
R21	2.56426	0.01997	0.00000	0.02622	0.02616
2.59043					
R22	2.65479	0.01820	0.00000	0.02780	0.02775
2.68253					
R23	2.02201	0.01300	0.00000	0.02530	0.02530
2.04731					
R24	2.56426	0.02505	0.00000	0.03479	0.03478
2.59904					
R25	2.02201	0.01264	0.00000	0.02460	0.02460
2.04661					
R26	2.02201	0.01391	0.00000	0.02361	0.02361
2.04561					
R27	3.30090	0.02586	0.00000	0.16940	0.16939
3.47030					
R28	2.02201	0.01755	0.00000	0.03416	0.03416
2.05617					
R29	2.37803	-0.04084	0.00000	-0.03996	-0.03996
2.33807					
A1	2.10209	-0.00163	0.00000	-0.01052	-0.01076
2.09134					
A2	2.09055	0.00170	0.00000	0.00881	0.00893
2.09947					
A3	2.09055	-0.00008	0.00000	0.00171	0.00183
2.09238					
A4	2.09402	0.00538	0.00000	0.01492	0.01484
2.10885					
A5	2.09458	-0.00095	0.00000	-0.00052	-0.00047
2.09411					
A6	2.09458	-0.00443	0.00000	-0.01441	-0.01436
2.08022					
A7	2.08707	0.00018	0.00000	0.00497	0.00510
2.09218					
A8	2.10025	-0.00026	0.00000	-0.00164	-0.00176
2.09849					
A9	2.09586	0.00008	0.00000	-0.00332	-0.00334
2.09252					
A10	2.08707	-0.01394	0.00000	-0.03779	-0.03759
2.04949					
A11	2.09586	-0.00730	0.00000	-0.01402	-0.01402
2.08184					
A12	2.10025	0.02124	0.00000	0.05181	0.05160
2.15186					
A13	2.09402	0.00708	0.00000	0.02332	0.02344
2.11745					
A14	2.09458	0.00022	0.00000	0.00335	0.00330
2.09788					

This journal is © The Royal Society of Chemistry 2014

A15	2.09458	-0.00730	0.00000	-0.02668	-0.02674
2.06785					
A16	2.10209	0.00293	0.00000	0.00510	0.00497
2.10706					
A17	2.09055	-0.00227	0.00000	-0.00576	-0.00569
2.08486					
A18	2.09055	-0.00066	0.00000	0.00065	0.00072
2.09127					
A19	2.09147	0.01072	0.00000	0.02739	0.02738
2.11884					
A20	2.09586	-0.00552	0.00000	-0.01434	-0.01433
2.08153					
A21	2.09586	-0.00520	0.00000	-0.01305	-0.01304
2.08281					
A22	2.09147	-0.00066	0.00000	0.00237	0.00248
2.09395					
A23	2.09586	0.00748	0.00000	0.00111	0.00103
2.09689					
A24	2.09586	-0.00682	0.00000	-0.00348	-0.00352
2.09234					
A25	2.09586	-0.00032	0.00000	-0.00398	-0.00401
2.09185					
A26	2.10025	0.00604	0.00000	0.02629	0.02624
2.12649					
A27	2.08707	-0.00571	0.00000	-0.02231	-0.02223
2.06485					
A28	2.09586	-0.00252	0.00000	-0.00843	-0.00850
2.08736					
A29	2.10025	0.00430	0.00000	0.00720	0.00718
2.10743					
A30	2.08707	-0.00178	0.00000	0.00124	0.00132
2.08839					
A31	2.09458	-0.00355	0.00000	-0.01279	-0.01277
2.08182					
A32	2.09402	0.00333	0.00000	0.01048	0.01043
2.10445					
A33	2.09458	0.00023	0.00000	0.00231	0.00233
2.09691					
A34	2.10209	-0.00181	0.00000	-0.00957	-0.00967
2.09242					
A35	2.09055	0.00112	0.00000	0.00563	0.00568
2.09623					
A36	2.09055	0.00069	0.00000	0.00394	0.00399
2.09454					
A37	2.10209	0.00227	0.00000	0.00637	0.00632
2.10841					
A38	2.09055	-0.00172	0.00000	-0.00554	-0.00551
2.08503					
A39	2.09055	-0.00055	0.00000	-0.00083	-0.00080
2.08974					
A40	2.09402	0.00371	0.00000	0.01379	0.01383
2.10785					

This journal is © The Royal Society of Chemistry 2014

```
   A41        2.09458  -0.01831   0.00000  -0.06373  -0.06374
2.03084
   A42        2.09458   0.01460   0.00000   0.04994   0.04991
2.14449
   A43        2.09440  -0.00882   0.00000  -0.03262  -0.03263
2.06177
   A44        2.09440   0.01979   0.00000   0.07379   0.07380
2.16820
   A45        2.09440  -0.01096   0.00000  -0.04117  -0.04117
2.05322
    D1        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D2       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
    D3       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
    D4        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D5        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D6       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
    D7       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
    D8        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D9        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D10       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D11        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D12        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D13        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D14       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D15        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D16        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D17        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D18        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D19        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D20       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D21        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
```

This journal is © The Royal Society of Chemistry 2014

D22	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D23	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D24	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D25	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D26	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D27	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D28	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D29	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D30	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D31	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D32	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D33	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D34	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D35	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D36	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D37	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D38	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D39	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D40	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D41	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D42	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D43	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D44	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D45	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D46	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D47	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159

This journal is © The Royal Society of Chemistry 2014

```
   D48        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D49       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D50        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D51        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D52        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D53        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D54        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D55       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D56        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D57        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D58        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D59        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D60        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D61        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D62       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D63       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D64        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D65        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D66       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D67        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D68        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.040841     0.000450     NO
 RMS     Force            0.010894     0.000300     NO
 Maximum Displacement     0.211170     0.001800     NO
 RMS     Displacement     0.049777     0.001200     NO
 Predicted change in Energy=-2.212739D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
```

This journal is © The Royal Society of Chemistry 2014

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.637126	-4.450856	0.011082
2	6	0	-5.268600	-4.416188	0.016053
3	6	0	-4.569819	-3.174921	0.014949
4	6	0	-5.301816	-1.944510	0.008571
5	6	0	-6.728745	-2.027357	0.003525
6	6	0	-7.373083	-3.239243	0.004745
7	6	0	-3.166320	-3.153922	0.020089
8	6	0	-4.588249	-0.707070	0.007529
9	6	0	-3.164754	-0.706944	0.012805
10	6	0	-2.453500	-1.945913	0.019133
11	6	0	-1.029347	-1.940857	0.024393
12	1	0	-0.496302	-2.883689	0.029176
13	6	0	-0.336232	-0.758204	0.023437
14	6	0	-1.040401	0.474350	0.017153
15	6	0	-2.415509	0.499859	0.011984
16	1	0	-2.623026	-4.090421	0.024890
17	1	0	-7.159488	-5.399449	0.011970
18	1	0	-4.703813	-5.340209	0.020896
19	1	0	-7.323764	-1.129136	-0.001356
20	1	0	-8.455503	-3.273682	0.000835
21	1	0	0.747137	-0.763268	0.027468
22	1	0	-0.485906	1.404653	0.016433
23	1	0	-2.986044	1.419782	0.007126
24	6	0	-5.339083	0.599354	0.000850
25	1	0	-6.426642	0.565993	-0.003084
26	8	0	-4.798953	1.712481	-0.000465

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.368975	0.000000			
3	C	2.429359	1.424443	0.000000		
4	C	2.839865	2.471913	1.431703	0.000000	
5	C	2.425242	2.799767	2.444994	1.429341	0.000000
6	C	1.417632	2.411261	2.804021	2.442641	1.372530
7	C	3.705214	2.452123	1.403665	2.454211	3.736347
8	C	4.267768	3.771008	2.467931	1.428438	2.514935
9	C	5.106296	4.264349	2.839916	2.469539	3.800739
10	C	4.876221	3.745271	2.447302	2.848336	4.276049
11	C	6.143896	4.909032	3.749393	4.272500	5.700093
12	H	6.337670	5.012340	4.083939	4.896473	6.291050
13	C	7.303225	6.140778	4.874818	5.105347	6.517313
14	C	7.455268	6.464907	5.076807	4.900062	6.214176
15	C	6.506277	5.683983	4.259703	3.782290	4.999090
16	H	4.030274	2.665570	2.151335	3.432364	4.594956
17	H	1.082908	2.131262	3.413930	3.922698	3.399501
18	H	2.128085	1.082970	2.169438	3.447976	3.882736

This journal is © The Royal Society of Chemistry 2014

19	H	3.391969	3.876689	3.430702	2.180185	1.077438
20	H	2.166180	3.385543	3.886964	3.422353	2.129560
21	H	8.253843	7.037972	5.838343	6.163240	7.582039
22	H	8.492616	7.533681	6.136028	5.865999	7.124037
23	H	6.913379	6.266473	4.860011	4.084270	5.088281
24	C	5.214369	5.016060	3.851898	2.544149	2.971663
25	H	5.021283	5.115032	4.176429	2.750999	2.610896
26	O	6.431620	6.146659	4.892794	3.691413	4.208385

		6	7	8	9	10
6	C	0.000000				
7	C	4.207656	0.000000			
8	C	3.763935	2.830039	0.000000		
9	C	4.911480	2.446990	1.423505	0.000000	
10	C	5.086768	1.402641	2.468201	1.428624	0.000000
11	C	6.475275	2.457275	3.766735	2.466301	1.424172
12	H	6.886010	2.683674	4.634886	3.443708	2.170288
13	C	7.461446	3.707948	4.252354	2.829006	2.427652
14	C	7.341239	4.205223	3.739394	2.430709	2.802592
15	C	6.209547	3.730134	2.485457	1.420472	2.446078
16	H	4.825760	1.082692	3.912731	3.426592	2.151207
17	H	2.170752	4.581249	5.350673	6.162589	5.837233
18	H	3.396958	2.672777	4.634599	4.882204	4.072488
19	H	2.110692	4.624344	2.767899	4.180408	4.938321
20	H	1.082974	5.290573	4.641465	5.880503	6.147141
21	H	8.489343	4.585895	5.335719	3.912324	3.412154
22	H	8.306570	5.288217	4.613964	3.411023	3.885579
23	H	6.399425	4.577274	2.662811	2.134229	3.407587
24	C	4.344191	4.336859	1.506832	2.536585	3.847766
25	H	3.921177	4.946514	2.236178	3.501505	4.700641
26	O	5.580837	5.133009	2.428721	2.919657	4.345730

		11	12	13	14	15
11	C	0.000000				
12	H	1.083094	0.000000			
13	C	1.370795	2.131512	0.000000		
14	C	2.415243	3.401855	1.419536	0.000000	
15	C	2.806902	3.889994	2.430277	1.375354	0.000000
16	H	2.675900	2.445235	4.041423	4.831345	4.594987
17	H	7.038511	7.122316	8.252158	8.482026	7.570150
18	H	5.005728	4.872136	6.330130	6.872387	6.272385
19	H	6.346593	7.049371	6.997414	6.484763	5.171534
20	H	7.544850	7.968800	8.500041	8.308534	7.121886
21	H	2.131343	2.458115	1.083389	2.174190	3.405593
22	H	3.389370	4.288374	2.168041	1.083019	2.131206
23	H	3.888812	4.971837	3.430071	2.163207	1.082493
24	C	5.002705	5.965310	5.183820	4.300530	2.925287
25	H	5.951122	6.860779	6.232760	5.387058	4.011706
26	O	5.249516	6.295908	5.101051	3.957270	2.674211

		16	17	18	19	20
16	H	0.000000				
17	H	4.721569	0.000000			
18	H	2.427274	2.456406	0.000000		
19	H	5.555793	4.273492	4.959615	0.000000	

This journal is © The Royal Society of Chemistry 2014

20	H	5.889433	2.489711	4.283236	2.424854	0.000000
21	H	4.735816	9.165650	7.117675	8.079241	9.538945
22	H	5.896032	9.530609	7.955120	7.292236	9.241295
23	H	5.522177	7.994972	6.974841	5.031190	7.207193
24	C	5.419552	6.268942	5.973473	2.631851	4.971165
25	H	6.012526	6.010306	6.152393	1.917888	4.342741
26	O	6.197497	7.493452	7.053364	3.801244	6.183218

		21	22	23	24	25
21	H	0.000000				
22	H	2.494073	0.000000			
23	H	4.324669	2.500200	0.000000		
24	C	6.236949	4.919560	2.491974	0.000000	
25	H	7.295956	5.999673	3.544965	1.088078	0.000000
26	O	6.073650	4.324050	1.836401	1.237252	1.990933

		26	
26	O	0.000000	

Stoichiometry C15H10O
Framework group C1[X(C15H10O)]
Deg. of freedom 72
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.794430	-0.922136	0.000003
2	6	0	2.645259	-1.666111	0.000001
3	6	0	1.367742	-1.036040	-0.000003
4	6	0	1.277336	0.392805	-0.000003
5	6	0	2.501911	1.129983	0.000000
6	6	0	3.717903	0.493429	0.000002
7	6	0	0.197423	-1.811041	-0.000003
8	6	0	-0.010226	1.011369	-0.000004
9	6	0	-1.185268	0.207851	-0.000004
10	6	0	-1.072908	-1.216347	-0.000003
11	6	0	-2.251276	-2.016169	0.000001
12	1	0	-2.158999	-3.095325	0.000002
13	6	0	-3.491027	-1.431280	0.000002
14	6	0	-3.605612	-0.016376	0.000003
15	6	0	-2.484982	0.780986	0.000000
16	1	0	0.277664	-2.890756	0.000000
17	1	0	4.761104	-1.410224	0.000005
18	1	0	2.700717	-2.747660	0.000005
19	1	0	2.485972	2.207304	0.000000
20	1	0	4.630788	1.076073	0.000003
21	1	0	-4.382394	-2.047068	0.000002
22	1	0	-4.588485	0.438476	0.000008
23	1	0	-2.533381	1.862396	0.000002
24	6	0	-0.127996	2.513592	0.000000
25	1	0	0.788523	3.100028	0.000002

```
  26          8             0      -1.202221    3.127459    0.000001
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9898137      0.4425688
0.3058266
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   324 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   324 basis functions,   552 primitive gaussians,   324 cartesian
basis functions
    54 alpha electrons       54 beta electrons
       nuclear repulsion energy       967.2688493806 Hartrees.
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   324 RedAO= T  NBF=   324
 NBsUse=   317 1.00D-06 NBFU=   317
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
```

This journal is © The Royal Society of Chemistry 2014

```
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -652.863150179     A.U. after   15 cycles
             Convg  =    0.5200D-08             -V/T =  2.0094
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.000762374   -0.002608513    0.000010641
    2          6          -0.004711738   -0.001479542   -0.000013093
    3          6           0.010086697   -0.007140387    0.000058520
    4          6          -0.003386790    0.012668214   -0.000050427
    5          6          -0.000733160   -0.003250646    0.000007099
    6          6           0.000657302    0.001606947   -0.000002274
    7          6          -0.004778919    0.008411865   -0.000042775
    8          6          -0.010481334    0.011088217   -0.000071948
    9          6          -0.007559698    0.005144596   -0.000043405
   10          6           0.001170380   -0.013147158    0.000043326
   11          6           0.003404845    0.003011241    0.000003800
   12          1           0.000348633   -0.003411546    0.000011535
   13          6           0.000644898   -0.000914783    0.000005106
   14          6          -0.002139456   -0.001503336   -0.000003306
   15          6           0.007914506    0.004876838    0.000014651
   16          1           0.001717169   -0.003334804    0.000016349
   17          1          -0.001473013   -0.002259629    0.000001217
   18          1           0.002932314   -0.001902833    0.000016649
   19          1          -0.002385932    0.002727831   -0.000016965
   20          1          -0.002779958    0.000312741   -0.000011289
   21          1           0.002605423    0.000239656    0.000008810
   22          1           0.001367643    0.002567959   -0.000002542
   23          1           0.010228056   -0.000923789    0.000040737
   24          6           0.027245272    0.001064382    0.000097910
   25          1          -0.008062551   -0.002931909   -0.000021154
   26          8          -0.022592964   -0.008911613   -0.000057172
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.027245272 RMS     0.005844105


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.016886277 RMS     0.003087071
 Search for a local minimum.
 Step number   2 out of a maximum of 152
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2
 Trust test= 9.66D-01 RLast= 3.00D-01 DXMaxT set to 4.24D-01
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.00237   0.00237   0.01521   0.02070
0.02070
     Eigenvalues ---    0.02084   0.02085   0.02088   0.02088
0.02093
     Eigenvalues ---    0.02097   0.02229   0.02231   0.02252
0.02257
     Eigenvalues ---    0.02349   0.02349   0.02374   0.02385
0.02424
     Eigenvalues ---    0.02432   0.02500   0.02504   0.07164
0.15862
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16027   0.16935
0.21969
     Eigenvalues ---    0.22000   0.22359   0.22612   0.22959
0.23570
     Eigenvalues ---    0.24464   0.24808   0.24987   0.25152
0.27057
     Eigenvalues ---    0.36509   0.36665   0.37230   0.37230
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37230   0.37230
0.37449
     Eigenvalues ---    0.37831   0.40936   0.41486   0.42910
0.42987
     Eigenvalues ---    0.43717   0.44607   0.45110   0.45332
0.45552
     Eigenvalues ---    0.45731   0.48301   0.51571   0.51597
0.52936
     Eigenvalues ---    0.56529
0.789561000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-3.95659437D-03.
 Quartic linear search produced a step of  0.41120.
 Iteration  1 RMS(Cart)=  0.02728064 RMS(Int)=  0.00253895
 Iteration  2 RMS(Cart)=  0.00259528 RMS(Int)=  0.00002823
 Iteration  3 RMS(Cart)=  0.00000475 RMS(Int)=  0.00002794
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00002794
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.58699   0.00197   0.00934  -0.00550   0.00379
2.59078
    R2        2.67894   0.00435   0.00993   0.00168   0.01155
2.69048
    R3        2.04640   0.00269   0.01003  -0.00116   0.00887
2.05527
    R4        2.69181   0.00525   0.01923  -0.00485   0.01439
2.70619
    R5        2.04652   0.00315   0.01008   0.00051   0.01058
2.05710
    R6        2.70553   0.01002   0.02623   0.00079   0.02709
2.73261
    R7        2.65254  -0.00173   0.00176  -0.00990  -0.00816
2.64438
    R8        2.70106   0.00416   0.02304  -0.01234   0.01076
2.71182
    R9        2.69936   0.00070   0.02101  -0.01990   0.00112
2.70048
   R10        2.59371   0.00254   0.01211  -0.00703   0.00507
2.59878
   R11        2.03606   0.00359   0.00578   0.00697   0.01275
2.04882
   R12        2.04652   0.00277   0.01008  -0.00092   0.00916
2.05569
   R13        2.65061  -0.00189   0.00096  -0.00806  -0.00712
2.64349
   R14        2.04599   0.00375   0.00986   0.00298   0.01284
2.05883
   R15        2.69003   0.00222   0.01718  -0.00500   0.01222
2.70225
   R16        2.84750  -0.01689  -0.02577  -0.04820  -0.07396
2.77354
   R17        2.69971   0.00939   0.02384   0.00599   0.02986
2.72957
   R18        2.68430   0.00631   0.01614   0.00517   0.02136
2.70567
   R19        2.69129   0.00478   0.01902  -0.00616   0.01287
2.70416
```

This journal is © The Royal Society of Chemistry 2014

R20	2.04675	0.00314	0.01017	0.00038	0.01055
2.05730					
R21	2.59043	0.00261	0.01076	-0.00681	0.00391
2.59433					
R22	2.68253	0.00381	0.01141	-0.00324	0.00813
2.69067					
R23	2.04731	0.00261	0.01040	-0.00189	0.00851
2.05582					
R24	2.59904	0.00151	0.01430	-0.01207	0.00223
2.60127					
R25	2.04661	0.00290	0.01012	-0.00045	0.00966
2.05627					
R26	2.04561	0.00344	0.00971	-0.00160	0.00810
2.05371					
R27	3.47030	0.01466	0.06965	0.16089	0.23053
3.70082					
R28	2.05617	0.00815	0.01405	0.01475	0.02879
2.08496					
R29	2.33807	-0.01366	-0.01643	-0.00690	-0.02334
2.31473					
A1	2.09134	-0.00088	-0.00442	-0.00276	-0.00730
2.08403					
A2	2.09947	0.00065	0.00367	0.00143	0.00515
2.10463					
A3	2.09238	0.00023	0.00075	0.00134	0.00215
2.09452					
A4	2.10885	0.00084	0.00610	-0.00181	0.00424
2.11310					
A5	2.09411	0.00112	-0.00019	0.01069	0.01052
2.10463					
A6	2.08022	-0.00196	-0.00591	-0.00888	-0.01476
2.06546					
A7	2.09218	-0.00011	0.00210	0.00014	0.00231
2.09448					
A8	2.09849	0.00072	-0.00073	0.00457	0.00380
2.10228					
A9	2.09252	-0.00061	-0.00137	-0.00471	-0.00610
2.08642					
A10	2.04949	-0.00249	-0.01546	0.00368	-0.01167
2.03781					
A11	2.08184	-0.00126	-0.00576	0.00372	-0.00205
2.07980					
A12	2.15186	0.00375	0.02122	-0.00741	0.01372
2.16557					
A13	2.11745	0.00100	0.00964	-0.00488	0.00481
2.12227					
A14	2.09788	-0.00001	0.00136	-0.00081	0.00052
2.09840					
A15	2.06785	-0.00099	-0.01099	0.00569	-0.00533
2.06252					
A16	2.10706	0.00165	0.00204	0.00563	0.00761
2.11468					

This journal is © The Royal Society of Chemistry 2014

A17	2.08486	-0.00041	-0.00234	0.00234	0.00003
2.08488					
A18	2.09127	-0.00124	0.00030	-0.00797	-0.00764
2.08363					
A19	2.11884	0.00277	0.01126	0.00291	0.01417
2.13301					
A20	2.08153	-0.00158	-0.00589	-0.00281	-0.00871
2.07282					
A21	2.08281	-0.00119	-0.00536	-0.00010	-0.00546
2.07735					
A22	2.09395	0.00100	0.00102	0.00483	0.00589
2.09984					
A23	2.09689	-0.00168	0.00042	-0.02852	-0.02817
2.06873					
A24	2.09234	0.00068	-0.00145	0.02369	0.02227
2.11462					
A25	2.09185	-0.00096	-0.00165	-0.00737	-0.00904
2.08281					
A26	2.12649	0.00198	0.01079	0.00795	0.01872
2.14520					
A27	2.06485	-0.00102	-0.00914	-0.00058	-0.00968
2.05517					
A28	2.08736	-0.00094	-0.00349	0.00063	-0.00288
2.08449					
A29	2.10743	0.00206	0.00295	0.00032	0.00323
2.11066					
A30	2.08839	-0.00112	0.00054	-0.00094	-0.00035
2.08804					
A31	2.08182	-0.00168	-0.00525	-0.00792	-0.01316
2.06866					
A32	2.10445	0.00054	0.00429	-0.00087	0.00339
2.10784					
A33	2.09691	0.00114	0.00096	0.00880	0.00977
2.10668					
A34	2.09242	0.00037	-0.00398	0.00218	-0.00187
2.09056					
A35	2.09623	0.00007	0.00234	0.00066	0.00303
2.09926					
A36	2.09454	-0.00044	0.00164	-0.00284	-0.00116
2.09337					
A37	2.10841	0.00135	0.00260	0.00437	0.00694
2.11535					
A38	2.08503	-0.00053	-0.00227	0.00017	-0.00208
2.08295					
A39	2.08974	-0.00081	-0.00033	-0.00454	-0.00486
2.08489					
A40	2.10785	-0.00012	0.00569	-0.00416	0.00157
2.10942					
A41	2.03084	-0.00287	-0.02621	0.01513	-0.01108
2.01976					
A42	2.14449	0.00299	0.02052	-0.01097	0.00951
2.15401					

A43	2.06177	-0.00554	-0.01342	-0.03256	-0.04599
2.01578					
A44	2.16820	0.00556	0.03035	0.01358	0.04396
2.21216					
A45	2.05322	-0.00002	-0.01693	0.01897	0.00203
2.05525					
D1	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D2	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D3	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D4	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D5	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D6	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D7	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D8	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D9	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D10	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D11	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D12	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D13	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D14	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D15	3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D16	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D17	3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D18	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D19	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D20	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D21	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D22	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D23	3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					

This journal is © The Royal Society of Chemistry 2014

D24	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D25	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D26	3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D27	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D28	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D29	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D30	3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D31	3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D32	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D33	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D34	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D35	3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D36	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D37	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D38	3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D39	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D40	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D41	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D42	-3.14159	0.00000	0.00000	-0.00001	-0.00001
3.14159					
D43	3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D44	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D45	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D46	3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D47	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D48	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D49	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					

```
   D50        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D51        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D52        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D53        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D54        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D55       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D56        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D57        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D58        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D59        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D60        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D61        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D62       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D63       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D64        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D65        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D66       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D67        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D68        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.016886     0.000450     NO
 RMS     Force            0.003087     0.000300     NO
 Maximum Displacement     0.203919     0.001800     NO
 RMS     Displacement     0.029537     0.001200     NO
 Predicted change in Energy=-3.539659D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
```

1	6	0	-6.643474	-4.453758	0.011069
2	6	0	-5.273119	-4.412625	0.016026
3	6	0	-4.571149	-3.164418	0.014909
4	6	0	-5.308152	-1.920310	0.008470
5	6	0	-6.739878	-2.017528	0.003454
6	6	0	-7.379409	-3.234988	0.004711
7	6	0	-3.172070	-3.137562	0.020015
8	6	0	-4.589446	-0.685159	0.007454
9	6	0	-3.159490	-0.682201	0.012746
10	6	0	-2.449230	-1.939920	0.019126
11	6	0	-1.018267	-1.944435	0.024445
12	1	0	-0.501406	-2.902584	0.029216
13	6	0	-0.312184	-0.767067	0.023554
14	6	0	-1.008289	0.474994	0.017273
15	6	0	-2.384032	0.521398	0.012035
16	1	0	-2.629588	-4.082375	0.024841
17	1	0	-7.168550	-5.406211	0.011961
18	1	0	-4.691361	-5.332690	0.020923
19	1	0	-7.347920	-1.119907	-0.001474
20	1	0	-8.466763	-3.266700	0.000775
21	1	0	0.775626	-0.779841	0.027625
22	1	0	-0.441566	1.403894	0.016606
23	1	0	-2.951593	1.448187	0.007170
24	6	0	-5.351421	0.569226	0.000892
25	1	0	-6.449117	0.458084	-0.002844
26	8	0	-4.893039	1.705128	-0.000789

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.370980	0.000000			
3	C	2.440684	1.432056	0.000000		
4	C	2.863818	2.492573	1.446036	0.000000	
5	C	2.438149	2.808564	2.453339	1.435032	0.000000
6	C	1.423742	2.413175	2.809165	2.453263	1.375213
7	C	3.712559	2.457684	1.399346	2.458593	3.739520
8	C	4.292014	3.789655	2.479338	1.429033	2.529739
9	C	5.134471	4.287599	2.855554	2.479855	3.821305
10	C	4.889901	3.753483	2.449889	2.859009	4.291379
11	C	6.159532	4.918923	3.756517	4.289982	5.722117
12	H	6.334940	5.004962	4.078182	4.906128	6.300994
13	C	7.326465	6.156382	4.887347	5.127367	6.548230
14	C	7.486518	6.486725	5.093064	4.922030	6.250118
15	C	6.549430	5.717642	4.285876	3.809518	5.041788
16	H	4.031054	2.664095	2.147651	3.442310	4.599841
17	H	1.087600	2.140067	3.431055	3.951279	3.415700
18	H	2.140879	1.088571	2.171610	3.467697	3.897054
19	H	3.407487	3.891927	3.448297	2.191210	1.084188
20	H	2.175683	3.393042	3.896982	3.433606	2.131330
21	H	8.278948	7.055818	5.854432	6.189780	7.616774
22	H	8.530872	7.561468	6.158160	5.893560	7.167638

23	H	6.961534	6.303862	4.888675	4.110978	5.134423
24	C	5.186509	4.982490	3.814331	2.489924	2.935834
25	H	4.915705	5.010701	4.080392	2.637932	2.492636
26	O	6.402815	6.129572	4.880199	3.649137	4.155599
		6	7	8	9	10
6	C	0.000000				
7	C	4.208495	0.000000			
8	C	3.779620	2.832560	0.000000		
9	C	4.931988	2.455405	1.429969	0.000000	
10	C	5.097458	1.398873	2.480945	1.444426	0.000000
11	C	6.490766	2.462202	3.786738	2.485600	1.430980
12	H	6.886074	2.680997	4.650755	3.463493	2.172750
13	C	7.485764	3.714594	4.278077	2.848591	2.437739
14	C	7.372605	4.211000	3.764404	2.442700	2.812138
15	C	6.250143	3.742868	2.513892	1.431777	2.462191
16	H	4.824860	1.089487	3.922043	3.441239	2.150041
17	H	2.181450	4.595507	5.379603	6.195873	5.855529
18	H	3.409724	2.669613	4.648668	4.896299	4.066700
19	H	2.115325	4.637793	2.792537	4.211263	4.966891
20	H	1.087823	5.296303	4.658110	5.903129	6.162093
21	H	8.516623	4.598174	5.365945	3.936355	3.427178
22	H	8.345839	5.299103	4.644258	3.426210	3.900232
23	H	6.444974	4.591064	2.689559	2.140515	3.425168
24	C	4.311009	4.300025	1.467696	2.524039	3.836516
25	H	3.808449	4.865000	2.182999	3.481686	4.663689
26	O	5.530535	5.139438	2.409504	2.950376	4.388504
		11	12	13	14	15
11	C	0.000000				
12	H	1.088677	0.000000			
13	C	1.372862	2.143891	0.000000		
14	C	2.419460	3.415422	1.423839	0.000000	
15	C	2.818829	3.907458	2.439842	1.376535	0.000000
16	H	2.677152	2.433327	4.044951	4.837177	4.610335
17	H	7.057622	7.121746	8.278379	8.516891	7.617623
18	H	4.997190	4.843677	6.326304	6.877080	6.292392
19	H	6.383183	7.074859	7.044623	6.537200	5.228217
20	H	7.564988	7.973726	8.529118	8.344422	7.165852
21	H	2.138771	2.477266	1.087892	2.181071	3.417148
22	H	3.397639	4.306912	2.174824	1.088131	2.133540
23	H	3.904860	4.993306	3.445882	2.173393	1.086778
24	C	5.009518	5.964638	5.213454	4.344185	2.967796
25	H	5.938600	6.831572	6.258086	5.440891	4.065605
26	O	5.322951	6.365403	5.205437	4.074904	2.774256
		16	17	18	19	20
16	H	0.000000				
17	H	4.728096	0.000000			
18	H	2.411268	2.478296	0.000000		
19	H	5.571317	4.290077	4.980497	0.000000	
20	H	5.893939	2.502597	4.303764	2.420854	0.000000
21	H	4.743650	9.193121	7.114522	8.130713	9.571151
22	H	5.906492	9.572349	7.965070	7.353069	9.285391
23	H	5.539956	8.047703	7.000520	5.091451	7.255846

This journal is © The Royal Society of Chemistry 2014

24	C	5.389466	6.245633	5.938746	2.615184	4.941628
25	H	5.933408	5.908279	6.051721	1.816013	4.236145
26	O	6.214423	7.466543	7.040741	3.742628	6.122955

		21	22	23	24	25
21	H	0.000000				
22	H	2.500075	0.000000			
23	H	4.342429	2.510436	0.000000		
24	C	6.273866	4.980320	2.555735	0.000000	
25	H	7.330095	6.081579	3.634979	1.103315	0.000000
26	O	6.189478	4.461687	1.958391	1.224904	1.994117

		26
26	O	0.000000

Stoichiometry C15H10O
Framework group C1[X(C15H10O)]
Deg. of freedom 72
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.789215	-0.971849	0.000000
2	6	0	-2.626104	-1.697631	0.000000
3	6	0	-1.349728	-1.048286	-0.000001
4	6	0	-1.273023	0.395714	-0.000001
5	6	0	-2.518309	1.108863	0.000000
6	6	0	-3.725675	0.450474	0.000001
7	6	0	-0.170632	-1.801879	0.000000
8	6	0	0.010037	1.024913	-0.000001
9	6	0	1.201574	0.234310	-0.000001
10	6	0	1.095067	-1.206184	0.000000
11	6	0	2.283296	-2.003565	0.000001
12	1	0	2.182000	-3.087519	0.000002
13	6	0	3.523808	-1.415448	0.000001
14	6	0	3.633408	0.004167	0.000000
15	6	0	2.514361	0.805778	-0.000001
16	1	0	-0.243212	-2.888945	0.000000
17	1	0	-4.754370	-1.473197	0.000001
18	1	0	-2.652276	-2.785887	0.000000
19	1	0	-2.526454	2.193020	0.000001
20	1	0	-4.648072	1.027141	0.000001
21	1	0	4.421911	-2.029385	0.000002
22	1	0	4.620155	0.462818	0.000000
23	1	0	2.556076	1.891756	-0.000001
24	6	0	0.071662	2.491315	-0.000001
25	1	0	-0.903392	3.007621	0.000000
26	8	0	1.083059	3.182304	0.000002

Rotational constants (GHZ): 0.9809021 0.4404608
0.3039681

This journal is © The Royal Society of Chemistry 2014

```
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   324 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   324 basis functions,   552 primitive gaussians,   324 cartesian
basis functions
    54 alpha electrons       54 beta electrons
       nuclear repulsion energy       964.6670972474 Hartrees.
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   324 RedAO= T  NBF=   324
 NBsUse=   317 1.00D-06 NBFU=   317
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
```

This journal is © The Royal Society of Chemistry 2014

```
 No special actions if energy rises.
 Restarting incremental Fock formation.
 SCF Done:  E(RB+HF-LYP) =  -652.867037406     A.U. after   21 cycles
            Convg  =    0.1938D-08             -V/T =  2.0097
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.000579816    0.000003179    0.000002165
    2          6          -0.000800898    0.000100199   -0.000003312
    3          6          -0.000347967   -0.001219184    0.000002350
    4          6          -0.000805296   -0.000142655   -0.000002542
    5          6          -0.000830747   -0.001341957    0.000000891
    6          6           0.000595442    0.000176400    0.000001675
    7          6          -0.000455027   -0.000081369   -0.000001397
    8          6           0.003570230   -0.003039074    0.000022183
    9          6           0.000060306   -0.001150338    0.000003666
   10          6           0.000750443    0.000745222    0.000000571
   11          6           0.000221823    0.000853622   -0.000001769
   12          1          -0.000448396    0.000513462   -0.000003192
   13          6          -0.000419569   -0.000633033    0.000000397
   14          6          -0.000709594    0.000532888   -0.000004255
   15          6          -0.003122106   -0.000506224   -0.000010107
   16          1          -0.000142429    0.000427725   -0.000001824
   17          1           0.000267317    0.000742747   -0.000001222
   18          1          -0.000125145    0.000672962   -0.000002463
   19          1          -0.000029933   -0.002428973    0.000007112
   20          1           0.000592058    0.000031031    0.000002104
   21          1          -0.000725437    0.000216727   -0.000003360
   22          1          -0.000295942   -0.000552772    0.000000572
   23          1           0.009403639   -0.001085270    0.000038091
   24          6          -0.003444447    0.000949664   -0.000015081
   25          1           0.000989446    0.001460289   -0.000000864
   26          8          -0.004327590    0.004754732   -0.000030389
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.009403639 RMS     0.001596186


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.006497581 RMS     0.001282260
 Search for a local minimum.
 Step number   3 out of a maximum of 152
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3
 Trust test= 1.10D+00 RLast= 2.68D-01 DXMaxT set to 6.00D-01
     Eigenvalues ---    0.00237   0.00237   0.01525   0.02070
0.02070
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02084   0.02085   0.02088   0.02088
0.02093
     Eigenvalues ---    0.02097   0.02230   0.02232   0.02253
0.02258
     Eigenvalues ---    0.02348   0.02350   0.02375   0.02389
0.02425
     Eigenvalues ---    0.02434   0.02501   0.02504   0.05084
0.15850
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16002   0.16294   0.17578
0.21883
     Eigenvalues ---    0.22002   0.22353   0.22589   0.22847
0.23464
     Eigenvalues ---    0.24346   0.24668   0.24956   0.25016
0.31115
     Eigenvalues ---    0.36350   0.37093   0.37230   0.37230
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37230   0.37347
0.37634
     Eigenvalues ---    0.38502   0.40458   0.41557   0.42964
0.43030
     Eigenvalues ---    0.43697   0.44912   0.45333   0.45534
0.45698
     Eigenvalues ---    0.46388   0.47706   0.51582   0.51652
0.52938
     Eigenvalues ---    0.57731
0.813301000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-1.15504778D-03.
 Quartic linear search produced a step of  0.04505.
 Iteration  1 RMS(Cart)=  0.01719071 RMS(Int)=  0.00011622
 Iteration  2 RMS(Cart)=  0.00015431 RMS(Int)=  0.00000717
 Iteration  3 RMS(Cart)=  0.00000003 RMS(Int)=  0.00000717
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.59078  -0.00212   0.00017  -0.00375  -0.00358
2.58719
    R2        2.69048  -0.00160   0.00052  -0.00272  -0.00221
2.68828
    R3        2.05527  -0.00078   0.00040  -0.00105  -0.00065
2.05462
    R4        2.70619  -0.00097   0.00065  -0.00024   0.00040
2.70660
    R5        2.05710  -0.00064   0.00048  -0.00049  -0.00002
2.05708
    R6        2.73261   0.00089   0.00122   0.00564   0.00688
2.73949
    R7        2.64438  -0.00129  -0.00037  -0.00432  -0.00468
2.63970
    R8        2.71182   0.00113   0.00048   0.00460   0.00509
2.71691
    R9        2.70048   0.00447   0.00005   0.01164   0.01169
2.71217
   R10        2.59878  -0.00111   0.00023  -0.00133  -0.00110
2.59767
   R11        2.04882  -0.00199   0.00057  -0.00420  -0.00362
2.04520
   R12        2.05569  -0.00059   0.00041  -0.00049  -0.00008
2.05561
   R13        2.64349  -0.00108  -0.00032  -0.00375  -0.00408
2.63941
   R14        2.05883  -0.00044   0.00058   0.00025   0.00083
2.05966
   R15        2.70225   0.00043   0.00055   0.00431   0.00484
2.70709
   R16        2.77354   0.00650  -0.00333   0.01704   0.01370
2.78724
   R17        2.72957  -0.00074   0.00135   0.00226   0.00360
2.73317
   R18        2.70567   0.00035   0.00096   0.00415   0.00510
2.71077
   R19        2.70416  -0.00098   0.00058  -0.00049   0.00009
2.70425
   R20        2.05730  -0.00066   0.00048  -0.00056  -0.00009
2.05721
```

This journal is © The Royal Society of Chemistry 2014

R21	2.59433	-0.00198	0.00018	-0.00355	-0.00337
2.59096					
R22	2.69067	-0.00144	0.00037	-0.00269	-0.00232
2.68835					
R23	2.05582	-0.00073	0.00038	-0.00092	-0.00054
2.05528					
R24	2.60127	-0.00144	0.00010	-0.00210	-0.00199
2.59928					
R25	2.05627	-0.00063	0.00044	-0.00055	-0.00011
2.05616					
R26	2.05371	-0.00268	0.00036	-0.00716	-0.00679
2.04692					
R27	3.70082	0.00502	0.01039	0.09180	0.10220
3.80302					
R28	2.08496	-0.00113	0.00130	-0.00010	0.00120
2.08616					
R29	2.31473	0.00404	-0.00105	0.00244	0.00139
2.31613					
A1	2.08403	-0.00042	-0.00033	-0.00419	-0.00453
2.07950					
A2	2.10463	0.00034	0.00023	0.00313	0.00337
2.10800					
A3	2.09452	0.00008	0.00010	0.00106	0.00116
2.09569					
A4	2.11310	0.00035	0.00019	0.00172	0.00190
2.11500					
A5	2.10463	0.00008	0.00047	0.00203	0.00251
2.10714					
A6	2.06546	-0.00044	-0.00067	-0.00375	-0.00441
2.06105					
A7	2.09448	0.00131	0.00010	0.00659	0.00669
2.10118					
A8	2.10228	-0.00173	0.00017	-0.00729	-0.00713
2.09516					
A9	2.08642	0.00042	-0.00027	0.00071	0.00043
2.08685					
A10	2.03781	-0.00281	-0.00053	-0.01296	-0.01347
2.02435					
A11	2.07980	-0.00089	-0.00009	-0.00219	-0.00230
2.07750					
A12	2.16557	0.00370	0.00062	0.01515	0.01577
2.18134					
A13	2.12227	0.00093	0.00022	0.00582	0.00604
2.12831					
A14	2.09840	0.00096	0.00002	0.00669	0.00670
2.10510					
A15	2.06252	-0.00188	-0.00024	-0.01250	-0.01275
2.04977					
A16	2.11468	0.00065	0.00034	0.00303	0.00337
2.11804					
A17	2.08488	-0.00031	0.00000	-0.00109	-0.00109
2.08380					

This journal is © The Royal Society of Chemistry 2014

A18	2.08363	-0.00034	-0.00034	-0.00193	-0.00228
2.08135					
A19	2.13301	0.00064	0.00064	0.00334	0.00398
2.13699					
A20	2.07282	-0.00023	-0.00039	-0.00125	-0.00164
2.07118					
A21	2.07735	-0.00041	-0.00025	-0.00209	-0.00234
2.07501					
A22	2.09984	-0.00122	0.00027	-0.00324	-0.00297
2.09688					
A23	2.06873	0.00351	-0.00127	0.00736	0.00612
2.07485					
A24	2.11462	-0.00228	0.00100	-0.00412	-0.00316
2.11146					
A25	2.08281	0.00070	-0.00041	0.00098	0.00058
2.08339					
A26	2.14520	0.00077	0.00084	0.00746	0.00828
2.15348					
A27	2.05517	-0.00147	-0.00044	-0.00844	-0.00886
2.04631					
A28	2.08449	0.00035	-0.00013	0.00041	0.00027
2.08476					
A29	2.11066	-0.00108	0.00015	-0.00489	-0.00473
2.10593					
A30	2.08804	0.00074	-0.00002	0.00448	0.00446
2.09250					
A31	2.06866	-0.00026	-0.00059	-0.00269	-0.00328
2.06538					
A32	2.10784	0.00021	0.00015	0.00109	0.00124
2.10908					
A33	2.10668	0.00005	0.00044	0.00160	0.00204
2.10873					
A34	2.09056	-0.00029	-0.00008	-0.00285	-0.00294
2.08762					
A35	2.09926	0.00036	0.00014	0.00297	0.00311
2.10237					
A36	2.09337	-0.00006	-0.00005	-0.00012	-0.00017
2.09320					
A37	2.11535	0.00046	0.00031	0.00286	0.00316
2.11851					
A38	2.08295	-0.00027	-0.00009	-0.00160	-0.00169
2.08126					
A39	2.08489	-0.00019	-0.00022	-0.00126	-0.00148
2.08341					
A40	2.10942	0.00035	0.00007	0.00286	0.00293
2.11235					
A41	2.01976	0.00347	-0.00050	0.02263	0.02212
2.04188					
A42	2.15401	-0.00383	0.00043	-0.02549	-0.02505
2.12896					
A43	2.01578	0.00117	-0.00207	0.00185	-0.00021
2.01557					

This journal is © The Royal Society of Chemistry 2014

A44	2.21216	0.00049	0.00198	0.01029	0.01224
2.22440					
A45	2.05525	-0.00166	0.00009	-0.01214	-0.01204
2.04321					
D1	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D2	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D3	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D4	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D5	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D6	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D7	3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D8	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D9	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D10	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D11	3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D12	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D13	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D14	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D15	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D16	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D17	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D18	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D19	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D20	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D21	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D22	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D23	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D24	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					

D25	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D26	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D27	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D28	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D29	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D30	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D31	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D32	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D33	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D34	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D35	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D36	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D37	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D38	-3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D39	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D40	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D41	0.00000	0.00000	0.00000	-0.00005	-0.00005	-0.00005
D42	3.14159	0.00000	0.00000	0.00006	0.00006	-3.14154
D43	-3.14159	0.00000	0.00000	-0.00005	-0.00005	3.14154
D44	0.00000	0.00000	0.00000	0.00005	0.00005	0.00005
D45	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D46	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D47	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D48	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D49	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D50	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

```
   D51        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D52       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D53        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D54        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D55        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D56        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D57        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D58        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D59       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D60        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D61        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D62       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D63       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D64        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D65        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D66        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D67        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D68        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.006498     0.000450     NO
 RMS     Force            0.001282     0.000300     NO
 Maximum Displacement     0.083002     0.001800     NO
 RMS     Displacement     0.017156     0.001200     NO
 Predicted change in Energy=-5.901899D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -6.635798   -4.467390    0.011138
```

2	6	0	-5.267859	-4.411617	0.016040
3	6	0	-4.576847	-3.157066	0.014866
4	6	0	-5.318378	-1.911416	0.008412
5	6	0	-6.751097	-2.031202	0.003461
6	6	0	-7.378676	-3.254209	0.004776
7	6	0	-3.180292	-3.127864	0.019953
8	6	0	-4.596376	-0.671027	0.007396
9	6	0	-3.163858	-0.672528	0.012707
10	6	0	-2.455858	-1.933706	0.019083
11	6	0	-1.024917	-1.948237	0.024428
12	1	0	-0.517955	-2.911608	0.029174
13	6	0	-0.310088	-0.778249	0.023595
14	6	0	-0.999004	0.466410	0.017338
15	6	0	-2.373250	0.524411	0.012074
16	1	0	-2.637523	-4.073016	0.024777
17	1	0	-7.153675	-5.423387	0.012065
18	1	0	-4.673965	-5.323885	0.020955
19	1	0	-7.377910	-1.148938	-0.001487
20	1	0	-8.465728	-3.293853	0.000867
21	1	0	0.777358	-0.796597	0.027678
22	1	0	-0.425835	1.391277	0.016710
23	1	0	-2.907671	1.466569	0.007291
24	6	0	-5.354189	0.594332	0.000822
25	1	0	-6.453170	0.489790	-0.002987
26	8	0	-4.902326	1.733636	-0.000944

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.369085	0.000000			
3	C	2.440542	1.432270	0.000000		
4	C	2.875519	2.500723	1.449675	0.000000	
5	C	2.438927	2.804733	2.448482	1.437726	0.000000
6	C	1.422574	2.407337	2.803531	2.459255	1.374628
7	C	3.706067	2.450709	1.396870	2.459938	3.735450
8	C	4.309481	3.800392	2.486127	1.435219	2.548120
9	C	5.143477	4.290410	2.858229	2.485321	3.835931
10	C	4.887895	3.747986	2.448514	2.862627	4.296373
11	C	6.150471	4.906207	3.752008	4.293649	5.726819
12	H	6.312590	4.981143	4.066332	4.903558	6.295064
13	C	7.322877	6.146618	4.885087	5.134907	6.561775
14	C	7.491053	6.482151	5.092205	4.930632	6.270952
15	C	6.564100	5.722163	4.290586	3.821917	5.069199
16	H	4.017701	2.652055	2.144770	3.443802	4.592488
17	H	1.087257	2.140093	3.431656	3.962609	3.416001
18	H	2.140670	1.088562	2.169002	3.472804	3.893140
19	H	3.400444	3.885576	3.446564	2.196165	1.082271
20	H	2.173922	3.387623	3.891311	3.437586	2.129378
21	H	8.272236	7.043661	5.851452	6.196870	7.629055
22	H	8.537427	7.557697	6.157786	5.902951	7.191834
23	H	7.007912	6.334322	4.915711	4.149976	5.196763
24	C	5.221462	5.006717	3.831116	2.506015	2.974019

This journal is © The Royal Society of Chemistry 2014

25	H	4.960564	5.042729	4.101277	2.655875	2.538544
26	O	6.438773	6.156138	4.901546	3.668731	4.194279
		6	7	8	9	10
6	C	0.000000				
7	C	4.200313	0.000000			
8	C	3.796582	2.835754	0.000000		
9	C	4.942655	2.455402	1.432529	0.000000	
10	C	5.096869	1.396717	2.485218	1.446331	0.000000
11	C	6.486617	2.457067	3.793003	2.490509	1.431025
12	H	6.869314	2.671121	4.653407	3.466201	2.170683
13	C	7.489705	3.709282	4.287660	2.855748	2.437095
14	C	7.385350	4.204382	3.772923	2.446180	2.807666
15	C	6.271549	3.740387	2.524160	1.434477	2.459515
16	H	4.811381	1.089924	3.925676	3.441002	2.147017
17	H	2.180829	4.588820	5.396733	6.203975	5.852129
18	H	3.405772	2.655855	4.653524	4.890359	4.051334
19	H	2.105281	4.640755	2.822306	4.240921	4.984263
20	H	1.087781	5.288076	4.674520	5.914500	6.161888
21	H	8.518291	4.593240	5.375239	3.943197	3.427358
22	H	8.361979	5.292417	4.652590	3.428714	3.895704
23	H	6.501973	4.602532	2.724159	2.154391	3.430181
24	C	4.348544	4.310561	1.474943	2.530342	3.845989
25	H	3.856702	4.878492	2.189815	3.488668	4.674647
26	O	5.568747	5.157520	2.424062	2.968515	4.408514
		11	12	13	14	15
11	C	0.000000				
12	H	1.088631	0.000000			
13	C	1.371077	2.143469	0.000000		
14	C	2.414797	3.412119	1.422611	0.000000	
15	C	2.816406	3.904951	2.440019	1.375479	0.000000
16	H	2.667430	2.416910	4.033911	4.826095	4.605034
17	H	7.045460	7.095218	8.271163	8.518787	7.630778
18	H	4.970971	4.805368	6.301288	6.858051	6.284579
19	H	6.403130	7.082862	7.077581	6.580285	5.277017
20	H	7.561541	7.957010	8.534825	8.360133	7.190101
21	H	2.138804	2.480143	1.087608	2.179623	3.416378
22	H	3.392833	4.303889	2.172623	1.088072	2.131643
23	H	3.899481	4.987951	3.433207	2.154861	1.083185
24	C	5.020738	5.973406	5.227567	4.357095	2.981781
25	H	5.950686	6.840857	6.272647	5.454255	4.080095
26	O	5.347067	6.387637	5.234388	4.103915	2.803323
		16	17	18	19	20
16	H	0.000000				
17	H	4.713735	0.000000			
18	H	2.389934	2.481722	0.000000		
19	H	5.569757	4.280349	4.974134	0.000000	
20	H	5.880105	2.501304	4.301034	2.404998	0.000000
21	H	4.732477	9.181978	7.086134	8.162928	9.574531
22	H	5.894924	9.576195	7.946070	7.401647	9.305405
23	H	5.546196	8.093212	7.016427	5.179189	7.318037
24	C	5.400462	6.281021	5.957214	2.671038	4.979925
25	H	5.948036	5.954545	6.079882	1.881642	4.285599

This journal is © The Royal Society of Chemistry 2014

```
   26  O    6.232752   7.502781   7.061248   3.799704   6.162262
                 21         22         23         24         25
   21  H    0.000000
   22  H    2.496916   0.000000
   23  H    4.324555   2.482995   0.000000
   24  C    6.287391   4.992399   2.597363   0.000000
   25  H    7.344132   6.094410   3.677604   1.103949   0.000000
   26  O    6.217854   4.489598   2.012472   1.225641   1.988033
                 26
   26  O    0.000000
 Stoichiometry    C15H10O
 Framework group  C1[X(C15H10O)]
 Deg. of freedom    72
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        3.793158   -0.979441    0.000003
    2          6             0        2.626036   -1.695135    0.000006
    3          6             0        1.353323   -1.038173    0.000002
    4          6             0        1.275276    0.409399   -0.000005
    5          6             0        2.531854    1.108016   -0.000008
    6          6             0        3.734316    0.441915   -0.000004
    7          6             0        0.177237   -1.791875    0.000005
    8          6             0       -0.015285    1.037336   -0.000009
    9          6             0       -1.204135    0.238103   -0.000006
   10          6             0       -1.089590   -1.203685    0.000001
   11          6             0       -2.269872   -2.012862    0.000004
   12          1             0       -2.154260   -3.095336    0.000009
   13          6             0       -3.515260   -1.439396    0.000001
   14          6             0       -3.636452   -0.021956   -0.000006
   15          6             0       -2.527469    0.791739   -0.000010
   16          1             0        0.252964   -2.879164    0.000010
   17          1             0        4.755778   -1.484903    0.000006
   18          1             0        2.640986   -2.783594    0.000011
   19          1             0        2.560956    2.189895   -0.000014
   20          1             0        4.659180    1.014536   -0.000007
   21          1             0       -4.408148   -2.060398    0.000003
   22          1             0       -4.627650    0.426852   -0.000010
   23          1             0       -2.608461    1.871892   -0.000016
   24          6             0       -0.090789    2.510346   -0.000017
   25          1             0        0.880133    3.035715    0.000030
   26          8             0       -1.100695    3.204815    0.000029
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9728322      0.4394465
0.3027077
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   324 symmetry adapted basis functions of A   symmetry.
```

This journal is © The Royal Society of Chemistry 2014

```
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   324 basis functions,   552 primitive gaussians,   324 cartesian
basis functions
    54 alpha electrons       54 beta electrons
       nuclear repulsion energy       963.1468996670 Hartrees.
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   324 RedAO= T  NBF=   324
 NBsUse=   317 1.00D-06 NBFU=   317
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Restarting incremental Fock formation.
```

This journal is © The Royal Society of Chemistry 2014

```
 SCF Done:  E(RB+HF-LYP) =  -652.867698926     A.U. after   20 cycles
             Convg  =    0.9007D-08             -V/T =  2.0098
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000244158    0.000070679   -0.000001096
    2          6           0.000632927    0.000236680    0.000001622
    3          6          -0.001855709    0.000861254   -0.000009658
    4          6           0.000042821   -0.000865868    0.000003084
    5          6           0.001145487    0.001150806    0.000000885
    6          6           0.000149889   -0.000335323    0.000001543
    7          6           0.000905728   -0.001534058    0.000007951
    8          6           0.002465196   -0.002265107    0.000018845
    9          6           0.000371491   -0.000651746    0.000003498
   10          6           0.000399985    0.002547762   -0.000006242
   11          6          -0.000295560   -0.000217056   -0.000000490
   12          1          -0.000276915    0.000544497   -0.000002661
   13          6           0.000260700   -0.000225979    0.000001634
   14          6           0.000224922    0.000596290   -0.000000947
   15          6          -0.003415429   -0.001545438   -0.000007738
   16          1          -0.000244114    0.000612302   -0.000002689
   17          1           0.000255481    0.000518693   -0.000000593
   18          1          -0.000290144    0.000542402   -0.000002716
   19          1           0.000328086    0.000515149   -0.000000211
   20          1           0.000541551    0.000169387    0.000001498
   21          1          -0.000550396    0.000037591   -0.000002149
   22          1          -0.000423509   -0.000416890   -0.000000327
   23          1           0.005064712   -0.000356281    0.000019732
   24          6          -0.004582817   -0.000507639   -0.000026592
   25          1           0.000544085   -0.000740614    0.000007930
   26          8          -0.001154310    0.001258508   -0.000004115
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.005064712 RMS     0.001122108


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.003298868 RMS     0.000764649
 Search for a local minimum.
 Step number   4 out of a maximum of 152
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  2  3  4
 Trust test= 1.12D+00 RLast= 1.17D-01 DXMaxT set to 6.00D-01
     Eigenvalues ---    0.00237   0.00237   0.01523   0.02070
0.02070
     Eigenvalues ---    0.02084   0.02085   0.02088   0.02088
0.02092
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02097   0.02229   0.02232   0.02253
0.02258
     Eigenvalues ---    0.02348   0.02350   0.02374   0.02386
0.02425
     Eigenvalues ---    0.02432   0.02501   0.02504   0.02799
0.15931
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16001   0.16007   0.16463   0.17199
0.21954
     Eigenvalues ---    0.22011   0.22468   0.22621   0.23121
0.23767
     Eigenvalues ---    0.24520   0.24957   0.25000   0.27035
0.31242
     Eigenvalues ---    0.36715   0.37188   0.37230   0.37230
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37233   0.37374
0.37629
     Eigenvalues ---    0.38275   0.41533   0.42593   0.42993
0.43606
     Eigenvalues ---    0.44611   0.45261   0.45335   0.45559
0.45720
     Eigenvalues ---    0.46599   0.51572   0.51635   0.52930
0.55339
     Eigenvalues ---    0.61367
0.809961000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---  1000.00000 1000.00000
 RFO step:  Lambda=-4.70441693D-04.
 Quartic linear search produced a step of  0.18151.
 Iteration  1 RMS(Cart)=  0.00904501 RMS(Int)=  0.00006106
 Iteration  2 RMS(Cart)=  0.00007213 RMS(Int)=  0.00000765
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000765
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58719   0.00005  -0.00065   0.00047  -0.00018
2.58701
    R2        2.68828  -0.00023  -0.00040   0.00032  -0.00008
2.68820
    R3        2.05462  -0.00058  -0.00012  -0.00086  -0.00098
2.05364
    R4        2.70660  -0.00106   0.00007  -0.00068  -0.00060
2.70599
    R5        2.05708  -0.00062   0.00000  -0.00081  -0.00081
2.05627
    R6        2.73949  -0.00205   0.00125  -0.00150  -0.00025
2.73924
    R7        2.63970   0.00086  -0.00085   0.00139   0.00055
2.64025
    R8        2.71691  -0.00237   0.00092  -0.00309  -0.00216
2.71474
    R9        2.71217  -0.00330   0.00212  -0.00482  -0.00270
2.70947
   R10        2.59767  -0.00048  -0.00020  -0.00010  -0.00030
2.59737
   R11        2.04520   0.00023  -0.00066   0.00084   0.00018
2.04538
   R12        2.05561  -0.00055  -0.00001  -0.00063  -0.00064
2.05496
   R13        2.63941   0.00092  -0.00074   0.00191   0.00118
2.64059
   R14        2.05966  -0.00065   0.00015  -0.00073  -0.00058
2.05908
   R15        2.70709  -0.00191   0.00088  -0.00173  -0.00088
2.70621
   R16        2.78724   0.00074   0.00249   0.00231   0.00478
2.79202
   R17        2.73317  -0.00148   0.00065   0.00007   0.00072
2.73389
   R18        2.71077  -0.00171   0.00093  -0.00116  -0.00024
2.71052
   R19        2.70425  -0.00081   0.00002  -0.00012  -0.00011
2.70414
   R20        2.05721  -0.00061  -0.00002  -0.00079  -0.00081
2.05641
   R21        2.59096  -0.00061  -0.00061  -0.00109  -0.00170
2.58926
```

This journal is © The Royal Society of Chemistry 2014

R22	2.68835	-0.00035	-0.00042	-0.00027	-0.00069
2.68766					
R23	2.05528	-0.00055	-0.00010	-0.00072	-0.00082
2.05447					
R24	2.59928	-0.00026	-0.00036	0.00033	-0.00004
2.59924					
R25	2.05616	-0.00058	-0.00002	-0.00073	-0.00075
2.05541					
R26	2.04692	-0.00093	-0.00123	-0.00375	-0.00497
2.04195					
R27	3.80302	0.00311	0.01855	0.08880	0.10737
3.91039					
R28	2.08616	-0.00047	0.00022	0.00068	0.00089
2.08705					
R29	2.31613	0.00150	0.00025	0.00054	0.00080
2.31693					
A1	2.07950	0.00009	-0.00082	-0.00012	-0.00095
2.07855					
A2	2.10800	-0.00002	0.00061	0.00070	0.00131
2.10931					
A3	2.09569	-0.00007	0.00021	-0.00057	-0.00036
2.09533					
A4	2.11500	-0.00039	0.00035	-0.00055	-0.00021
2.11479					
A5	2.10714	0.00025	0.00046	0.00198	0.00244
2.10958					
A6	2.06105	0.00014	-0.00080	-0.00143	-0.00223
2.05882					
A7	2.10118	-0.00043	0.00122	-0.00092	0.00029
2.10147					
A8	2.09516	0.00084	-0.00129	0.00271	0.00141
2.09657					
A9	2.08685	-0.00041	0.00008	-0.00178	-0.00170
2.08515					
A10	2.02435	0.00165	-0.00244	0.00292	0.00048
2.02483					
A11	2.07750	0.00062	-0.00042	0.00157	0.00114
2.07864					
A12	2.18134	-0.00227	0.00286	-0.00449	-0.00162
2.17972					
A13	2.12831	-0.00074	0.00110	-0.00196	-0.00086
2.12745					
A14	2.10510	-0.00021	0.00122	-0.00061	0.00061
2.10571					
A15	2.04977	0.00095	-0.00231	0.00257	0.00025
2.05003					
A16	2.11804	-0.00019	0.00061	0.00064	0.00125
2.11929					
A17	2.08380	0.00025	-0.00020	0.00092	0.00072
2.08452					
A18	2.08135	-0.00007	-0.00041	-0.00155	-0.00197
2.07938					

This journal is © The Royal Society of Chemistry 2014

A19	2.13699	-0.00075	0.00072	-0.00015	0.00057
2.13756					
A20	2.07118	0.00047	-0.00030	0.00078	0.00049
2.07167					
A21	2.07501	0.00028	-0.00042	-0.00063	-0.00106
2.07396					
A22	2.09688	0.00087	-0.00054	0.00199	0.00146
2.09833					
A23	2.07485	-0.00235	0.00111	-0.01211	-0.01096
2.06389					
A24	2.11146	0.00148	-0.00057	0.01012	0.00950
2.12096					
A25	2.08339	-0.00007	0.00011	-0.00148	-0.00136
2.08203					
A26	2.15348	-0.00015	0.00150	0.00444	0.00592
2.15940					
A27	2.04631	0.00021	-0.00161	-0.00296	-0.00455
2.04176					
A28	2.08476	-0.00026	0.00005	-0.00014	-0.00010
2.08466					
A29	2.10593	-0.00008	-0.00086	-0.00228	-0.00313
2.10280					
A30	2.09250	0.00034	0.00081	0.00243	0.00323
2.09573					
A31	2.06538	0.00009	-0.00060	-0.00126	-0.00186
2.06352					
A32	2.10908	-0.00018	0.00023	0.00031	0.00053
2.10961					
A33	2.10873	0.00008	0.00037	0.00096	0.00133
2.11005					
A34	2.08762	-0.00031	-0.00053	-0.00243	-0.00297
2.08465					
A35	2.10237	0.00018	0.00056	0.00182	0.00239
2.10475					
A36	2.09320	0.00013	-0.00003	0.00061	0.00058
2.09378					
A37	2.11851	0.00005	0.00057	0.00189	0.00246
2.12097					
A38	2.08126	0.00011	-0.00031	0.00000	-0.00030
2.08096					
A39	2.08341	-0.00017	-0.00027	-0.00189	-0.00216
2.08125					
A40	2.11235	-0.00012	0.00053	0.00077	0.00130
2.11365					
A41	2.04188	0.00186	0.00401	0.01637	0.02037
2.06225					
A42	2.12896	-0.00174	-0.00455	-0.01715	-0.02167
2.10729					
A43	2.01557	0.00005	-0.00004	-0.00479	-0.00482
2.01075					
A44	2.22440	-0.00174	0.00222	-0.00095	0.00124
2.22565					

This journal is © The Royal Society of Chemistry 2014

A45	2.04321	0.00169	-0.00218	0.00574	0.00357	2.04678
D1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D2	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D3	3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D4	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D6	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D7	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D10	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D11	-3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D12	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D14	3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D15	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D16	0.00000	0.00000	0.00000	0.00001	0.00001	0.00001
D17	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D18	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D19	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D20	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D21	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D22	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D23	-3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D24	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D25	0.00000	0.00000	0.00000	-0.00001	-0.00001	-0.00001

This journal is © The Royal Society of Chemistry 2014

D26	-3.14159	0.00000	0.00000	-0.00001	-0.00001	3.14158
D27	3.14159	0.00000	0.00000	-0.00001	-0.00001	3.14158
D28	0.00000	0.00000	0.00000	-0.00001	-0.00001	-0.00001
D29	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D30	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D31	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D32	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D33	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D34	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D35	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D36	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D37	0.00000	0.00000	0.00000	0.00001	0.00001	0.00001
D38	3.14159	0.00000	0.00000	0.00001	0.00001	-3.14159
D39	3.14159	0.00000	0.00000	0.00001	0.00001	-3.14158
D40	0.00000	0.00000	0.00000	0.00001	0.00001	0.00001
D41	-0.00005	0.00000	-0.00001	0.00144	0.00143	0.00138
D42	-3.14154	0.00000	0.00001	-0.00155	-0.00154	3.14011
D43	3.14154	0.00000	-0.00001	0.00144	0.00143	-3.14021
D44	0.00005	0.00000	0.00001	-0.00155	-0.00154	-0.00149
D45	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D46	-3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D47	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D48	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D49	3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D50	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D51	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

```
   D52       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D53        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D54       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D55        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D56        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D57        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D58       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D59       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D60        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D61        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D62        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D63        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D64        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D65        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D66        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D67       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D68        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.003299     0.000450     NO
 RMS     Force            0.000765     0.000300     NO
 Maximum Displacement     0.056882     0.001800     NO
 RMS     Displacement     0.009026     0.001200     NO
 Predicted change in Energy=-2.453425D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -6.635479   -4.465264    0.011141
    2          6             0       -5.267605   -4.410248    0.016111
    3          6             0       -4.576314   -3.156217    0.014857
```

This journal is © The Royal Society of Chemistry 2014

4	6	0	-5.316984	-1.910208	0.008246
5	6	0	-6.748694	-2.028298	0.003231
6	6	0	-7.376514	-3.251005	0.004628
7	6	0	-3.179499	-3.125518	0.020015
8	6	0	-4.596327	-0.670691	0.007143
9	6	0	-3.164273	-0.669383	0.012530
10	6	0	-2.455336	-1.930468	0.019070
11	6	0	-1.024495	-1.948765	0.024510
12	1	0	-0.522060	-2.914022	0.029364
13	6	0	-0.306444	-0.781809	0.023629
14	6	0	-0.994942	0.462667	0.017217
15	6	0	-2.369009	0.524312	0.011857
16	1	0	-2.635417	-4.069561	0.024962
17	1	0	-7.154886	-5.419840	0.012121
18	1	0	-4.672227	-5.321034	0.021146
19	1	0	-7.375116	-1.145636	-0.001832
20	1	0	-8.463309	-3.288223	0.000660
21	1	0	0.780556	-0.800987	0.027777
22	1	0	-0.421524	1.386913	0.016536
23	1	0	-2.879111	1.476872	0.007009
24	6	0	-5.369922	0.588053	0.000356
25	1	0	-6.467529	0.465583	-0.002019
26	8	0	-4.932427	1.733406	-0.000078

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.368989	0.000000			
3	C	2.440037	1.431950	0.000000		
4	C	2.875195	2.500540	1.449543	0.000000	
5	C	2.439607	2.804903	2.447769	1.436581	0.000000
6	C	1.422533	2.406548	2.801822	2.457521	1.374472
7	C	3.706588	2.451680	1.397161	2.458853	3.734076
8	C	4.307777	3.799340	2.485619	1.433789	2.544759
9	C	5.143732	4.291630	2.859756	2.484719	3.833381
10	C	4.888644	3.749423	2.449698	2.861740	4.294502
11	C	6.149479	4.905400	3.751460	4.292693	5.724791
12	H	6.307185	4.975849	4.061508	4.898917	6.289370
13	C	7.322888	6.146442	4.885661	5.136052	6.561764
14	C	7.490006	6.480814	5.091419	4.930584	6.269830
15	C	6.564955	5.722916	4.291678	3.823278	5.069273
16	H	4.019610	2.654159	2.145082	3.442947	4.591979
17	H	1.086739	2.140356	3.431186	3.961744	3.415792
18	H	2.141682	1.088132	2.166950	3.471255	3.892833
19	H	3.401053	3.885823	3.446159	2.195582	1.082368
20	H	2.174051	3.386990	3.889262	3.434872	2.127751
21	H	8.271926	7.043234	5.851779	6.197640	7.628663
22	H	8.535880	7.555897	6.156486	5.902255	7.190058
23	H	7.029886	6.353202	4.934174	4.173193	5.221102
24	C	5.209391	4.999373	3.827477	2.498834	2.957416
25	H	4.933724	5.021342	4.085880	2.639743	2.509686
26	O	6.428376	6.152812	4.902596	3.663861	4.177230

This journal is © The Royal Society of Chemistry 2014

		6	7	8	9	10
6	C	0.000000				
7	C	4.198918	0.000000			
8	C	3.793081	2.834386	0.000000		
9	C	4.940425	2.456194	1.432064	0.000000	
10	C	5.095293	1.397339	2.484154	1.446711	0.000000
11	C	6.484163	2.455364	3.793647	2.493113	1.430969
12	H	6.862777	2.665859	4.651095	3.466985	2.169111
13	C	7.488870	3.707753	4.291354	2.860062	2.436633
14	C	7.383493	4.200877	3.775523	2.446949	2.803542
15	C	6.271218	3.738746	2.527647	1.434348	2.456309
16	H	4.811283	1.089618	3.924003	3.441083	2.146667
17	H	2.180143	4.589954	5.394504	6.204179	5.853335
18	H	3.405651	2.654907	4.650984	4.889975	4.050993
19	H	2.105379	4.639354	2.819100	4.237714	4.982031
20	H	1.087440	5.286350	4.669590	5.910858	6.159511
21	H	8.517094	4.591899	5.378500	3.947053	3.427360
22	H	8.359564	5.288523	4.654332	3.427980	3.891198
23	H	6.525293	4.612201	2.749701	2.165123	3.433614
24	C	4.331835	4.311490	1.477474	2.538932	3.852026
25	H	3.826137	4.869048	2.189201	3.492829	4.673243
26	O	5.551390	5.165491	2.427487	2.983273	4.422705

		11	12	13	14	15
11	C	0.000000				
12	H	1.088203	0.000000			
13	C	1.370177	2.143095	0.000000		
14	C	2.411624	3.409661	1.422248	0.000000	
15	C	2.814959	3.903034	2.441366	1.375460	0.000000
16	H	2.663240	2.408645	4.029074	4.819990	4.601610
17	H	7.044871	7.090403	8.271193	8.517560	7.631354
18	H	4.967712	4.797673	6.297987	6.853732	6.282752
19	H	6.401258	7.077609	7.078075	6.579789	5.277312
20	H	7.558484	7.950113	8.533293	8.357389	7.188605
21	H	2.139068	2.482282	1.087176	2.179294	3.417079
22	H	3.389748	4.302129	2.171785	1.087677	2.129977
23	H	3.895498	4.983588	3.423527	2.139816	1.080554
24	C	5.031775	5.980563	5.245557	4.376809	3.001611
25	H	5.954528	6.838956	6.286145	5.472622	4.098964
26	O	5.369443	6.407089	5.265604	4.137495	2.834283

		16	17	18	19	20
16	H	0.000000				
17	H	4.716887	0.000000			
18	H	2.390564	2.484641	0.000000		
19	H	5.569093	4.279897	4.973941	0.000000	
20	H	5.880085	2.501179	4.301749	2.403092	0.000000
21	H	4.727838	9.181791	7.082634	8.163004	9.572675
22	H	5.888506	9.574450	7.941351	7.400445	9.302014
23	H	5.551813	8.114612	7.030434	5.204968	7.340943
24	C	5.401063	6.267457	5.950169	2.650752	4.959290
25	H	5.937452	5.925443	6.058761	1.849255	4.251377
26	O	6.241098	7.490555	7.059269	3.775661	6.138720

		21	22	23	24	25

```
   21  H    0.000000
   22  H    2.496404   0.000000
   23  H    4.310712   2.459252   0.000000
   24  C    6.305438   5.012493   2.644651   0.000000
   25  H    7.357976   6.115829   3.728207   1.104421   0.000000
   26  O    6.249967   4.524221   2.069291   1.226065   1.990959
                 26
   26  O    0.000000
 Stoichiometry    C15H10O
 Framework group  C1[X(C15H10O)]
 Deg. of freedom    72
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -3.786941   -0.992456    0.000091
    2          6             0       -2.617769   -1.704613    0.000167
    3          6             0       -1.347443   -1.043741    0.000050
    4          6             0       -1.273600    0.403919   -0.000154
    5          6             0       -2.530862    1.098943   -0.000225
    6          6             0       -3.730993    0.428976   -0.000107
    7          6             0       -0.167653   -1.792177    0.000136
    8          6             0        0.013129    1.036437   -0.000271
    9          6             0        1.205968    0.244008   -0.000174
   10          6             0        1.097355   -1.198619    0.000032
   11          6             0        2.278321   -2.006697    0.000129
   12          1             0        2.161724   -3.088635    0.000284
   13          6             0        3.522675   -1.433138    0.000030
   14          6             0        3.639099   -0.015664   -0.000173
   15          6             0        2.529414    0.797041   -0.000272
   16          1             0       -0.237827   -2.879533    0.000292
   17          1             0       -4.748253   -1.499289    0.000181
   18          1             0       -2.626813   -2.792708    0.000320
   19          1             0       -2.563243    2.180826   -0.000373
   20          1             0       -4.656320    1.000199   -0.000168
   21          1             0        4.416922   -2.051423    0.000103
   22          1             0        4.628568    0.435993   -0.000253
   23          1             0        2.632593    1.872658   -0.000430
   24          6             0        0.066621    2.512943   -0.000493
   25          1             0       -0.914942    3.019184    0.000828
   26          8             0        1.065457    3.223971    0.000828
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9693729      0.4398903
0.3025821
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   324 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
```

This journal is © The Royal Society of Chemistry 2014

```
 Two-electron integral symmetry is turned on.
   324 basis functions,   552 primitive gaussians,   324 cartesian
basis functions
    54 alpha electrons       54 beta electrons
       nuclear repulsion energy       962.9368376424 Hartrees.
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   324 RedAO= T  NBF=   324
 NBsUse=   317 1.00D-06 NBFU=   317
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -652.868001709     A.U. after   19 cycles
             Convg  =    0.7972D-08             -V/T =  2.0098
             S**2   =   0.0000
```

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000113166	0.000434049	-0.000002595
2	6	0.000850964	0.000323712	0.000002943
3	6	-0.001355072	0.001179579	-0.000001748
4	6	0.000661452	-0.001635453	-0.000001543
5	6	0.000340845	0.000548096	-0.000002792
6	6	-0.000069314	-0.000208483	0.000000460
7	6	0.000607891	-0.001195184	0.000004842
8	6	0.001048909	-0.000711256	-0.000079304
9	6	0.000541743	-0.000056414	-0.000002832
10	6	-0.000264017	0.001862172	-0.000001777
11	6	-0.000700616	-0.000625284	-0.000000205
12	1	-0.000054146	0.000326919	-0.000000987
13	6	0.000084539	0.000308505	-0.000000452
14	6	0.000607778	0.000227141	0.000001064
15	6	-0.001877358	-0.001483225	-0.000009386
16	1	-0.000202249	0.000406715	-0.000003250
17	1	0.000171105	0.000180325	0.000000174
18	1	-0.000363442	0.000129889	-0.000001405
19	1	0.000225094	-0.000079150	-0.000002362
20	1	0.000290292	-0.000023414	0.000001417
21	1	-0.000291192	-0.000055884	-0.000000753
22	1	-0.000276239	-0.000195042	-0.000000403
23	1	0.001391084	0.000291004	0.000006242
24	6	-0.002369886	0.000293199	0.000308824
25	1	0.001358466	0.000222458	-0.000101362
26	8	-0.000243464	-0.000464976	-0.000112809

Cartesian Forces: Max 0.002369886 RMS 0.000651339

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Internal Forces: Max 0.001680005 RMS 0.000359109
Search for a local minimum.
Step number 5 out of a maximum of 152
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points 2 3 4 5
Trust test= 1.23D+00 RLast= 1.14D-01 DXMaxT set to 6.00D-01
Eigenvalues --- 0.00236 0.00237 0.01524 0.02070
0.02070
Eigenvalues --- 0.02084 0.02085 0.02088 0.02088
0.02092
Eigenvalues --- 0.02097 0.02229 0.02231 0.02253
0.02258
Eigenvalues --- 0.02348 0.02350 0.02374 0.02383
0.02425

```
     Eigenvalues ---    0.02426   0.02431   0.02501   0.02504
0.15974
     Eigenvalues ---    0.15998   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16002   0.16057   0.16465   0.16809
0.21981
     Eigenvalues ---    0.22018   0.22420   0.22621   0.23020
0.23725
     Eigenvalues ---    0.24491   0.24953   0.25086   0.26399
0.31047
     Eigenvalues ---    0.36821   0.37209   0.37230   0.37230
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37317   0.37396
0.37552
     Eigenvalues ---    0.37905   0.41669   0.42553   0.42984
0.43623
     Eigenvalues ---    0.44590   0.45000   0.45335   0.45588
0.45768
     Eigenvalues ---    0.46524   0.51573   0.51607   0.52961
0.55885
     Eigenvalues ---    0.58696
0.812781000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-6.91346829D-05.
 Quartic linear search produced a step of  0.29678.
 Iteration  1 RMS(Cart)=  0.00970593 RMS(Int)=  0.00034583
```

This journal is © The Royal Society of Chemistry 2014

```
 Iteration  2 RMS(Cart)=  0.00028723 RMS(Int)=  0.00020738
 Iteration  3 RMS(Cart)=  0.00000022 RMS(Int)=  0.00020738
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58701  -0.00011  -0.00005  -0.00018  -0.00024
2.58678
    R2        2.68820  -0.00043  -0.00002  -0.00092  -0.00095
2.68725
    R3        2.05364  -0.00024  -0.00029  -0.00037  -0.00066
2.05298
    R4        2.70599  -0.00081  -0.00018  -0.00150  -0.00168
2.70431
    R5        2.05627  -0.00031  -0.00024  -0.00057  -0.00081
2.05546
    R6        2.73924  -0.00168  -0.00007  -0.00322  -0.00329
2.73595
    R7        2.64025  -0.00001   0.00016  -0.00039  -0.00023
2.64002
    R8        2.71474  -0.00079  -0.00064  -0.00060  -0.00124
2.71350
    R9        2.70947  -0.00081  -0.00080  -0.00004  -0.00084
2.70863
   R10        2.59737  -0.00030  -0.00009  -0.00028  -0.00037
2.59701
   R11        2.04538  -0.00019   0.00005  -0.00086  -0.00081
2.04457
   R12        2.05496  -0.00029  -0.00019  -0.00052  -0.00071
2.05425
   R13        2.64059   0.00021   0.00035   0.00021   0.00056
2.64115
   R14        2.05908  -0.00045  -0.00017  -0.00102  -0.00119
2.05788
   R15        2.70621  -0.00093  -0.00026  -0.00142  -0.00169
2.70452
   R16        2.79202   0.00038   0.00142   0.00150   0.00291
2.79493
   R17        2.73389  -0.00112   0.00021  -0.00211  -0.00190
2.73198
   R18        2.71052  -0.00108  -0.00007  -0.00196  -0.00204
2.70848
   R19        2.70414  -0.00076  -0.00003  -0.00146  -0.00149
2.70265
   R20        2.05641  -0.00031  -0.00024  -0.00058  -0.00082
2.05558
   R21        2.58926  -0.00011  -0.00050   0.00011  -0.00039
2.58887
   R22        2.68766  -0.00042  -0.00020  -0.00077  -0.00098
2.68668
   R23        2.05447  -0.00029  -0.00024  -0.00053  -0.00077
2.05370
```

This journal is © The Royal Society of Chemistry 2014

R24	2.59924	0.00012	-0.00001	0.00064	0.00063
2.59987					
R25	2.05541	-0.00031	-0.00022	-0.00059	-0.00081
2.05460					
R26	2.04195	-0.00010	-0.00148	0.00012	-0.00135
2.04060					
R27	3.91039	0.00052	0.03187	0.00644	0.03831
3.94871					
R28	2.08705	-0.00138	0.00026	-0.00422	-0.00396
2.08309					
R29	2.31693	-0.00040	0.00024	-0.00105	-0.00081
2.31612					
A1	2.07855	0.00015	-0.00028	0.00086	0.00058
2.07913					
A2	2.10931	-0.00013	0.00039	-0.00087	-0.00048
2.10882					
A3	2.09533	-0.00001	-0.00011	0.00001	-0.00009
2.09523					
A4	2.11479	-0.00022	-0.00006	-0.00076	-0.00082
2.11397					
A5	2.10958	-0.00013	0.00072	-0.00146	-0.00073
2.10884					
A6	2.05882	0.00035	-0.00066	0.00221	0.00155
2.06037					
A7	2.10147	0.00002	0.00009	0.00039	0.00047
2.10194					
A8	2.09657	0.00000	0.00042	-0.00076	-0.00034
2.09623					
A9	2.08515	-0.00002	-0.00051	0.00037	-0.00013
2.08502					
A10	2.02483	0.00060	0.00014	0.00083	0.00098
2.02580					
A11	2.07864	0.00031	0.00034	0.00069	0.00103
2.07967					
A12	2.17972	-0.00092	-0.00048	-0.00153	-0.00201
2.17771					
A13	2.12745	-0.00027	-0.00026	-0.00039	-0.00064
2.12680					
A14	2.10571	-0.00001	0.00018	0.00029	0.00047
2.10619					
A15	2.05003	0.00028	0.00007	0.00010	0.00017
2.05020					
A16	2.11929	-0.00028	0.00037	-0.00093	-0.00056
2.11872					
A17	2.08452	0.00011	0.00021	-0.00001	0.00020
2.08472					
A18	2.07938	0.00017	-0.00058	0.00094	0.00036
2.07974					
A19	2.13756	-0.00051	0.00017	-0.00173	-0.00156
2.13600					
A20	2.07167	0.00028	0.00014	0.00097	0.00111
2.07278					

A21	2.07396	0.00023	-0.00031	0.00076	0.00044
2.07440					
A22	2.09833	0.00019	0.00043	-0.00013	0.00031
2.09864					
A23	2.06389	-0.00039	-0.00325	0.00071	-0.00252
2.06137					
A24	2.12096	0.00020	0.00282	-0.00058	0.00221
2.12318					
A25	2.08203	-0.00023	-0.00040	-0.00093	-0.00133
2.08070					
A26	2.15940	0.00017	0.00176	0.00143	0.00318
2.16257					
A27	2.04176	0.00006	-0.00135	-0.00051	-0.00185
2.03991					
A28	2.08466	0.00027	-0.00003	0.00171	0.00168
2.08634					
A29	2.10280	-0.00059	-0.00093	-0.00287	-0.00380
2.09900					
A30	2.09573	0.00033	0.00096	0.00116	0.00211
2.09784					
A31	2.06352	0.00016	-0.00055	0.00083	0.00028
2.06380					
A32	2.10961	-0.00011	0.00016	-0.00027	-0.00012
2.10949					
A33	2.11005	-0.00005	0.00039	-0.00056	-0.00017
2.10989					
A34	2.08465	-0.00018	-0.00088	-0.00054	-0.00142
2.08323					
A35	2.10475	0.00002	0.00071	-0.00023	0.00048
2.10523					
A36	2.09378	0.00016	0.00017	0.00077	0.00094
2.09472					
A37	2.12097	-0.00012	0.00073	-0.00028	0.00045
2.12142					
A38	2.08096	0.00019	-0.00009	0.00095	0.00086
2.08182					
A39	2.08125	-0.00007	-0.00064	-0.00067	-0.00131
2.07994					
A40	2.11365	0.00002	0.00039	0.00043	0.00082
2.11447					
A41	2.06225	0.00095	0.00605	0.00517	0.01121
2.07346					
A42	2.10729	-0.00098	-0.00643	-0.00561	-0.01203
2.09526					
A43	2.01075	0.00044	-0.00143	0.00306	0.00022
2.01097					
A44	2.22565	-0.00073	0.00037	-0.00183	-0.00290
2.22275					
A45	2.04678	0.00029	0.00106	-0.00099	-0.00136
2.04543					
D1	0.00000	0.00000	0.00000	0.00001	0.00001
0.00001					

This journal is © The Royal Society of Chemistry 2014

D2	3.14159	0.00000	0.00000	0.00004	0.00004	-3.14156
D3	-3.14159	0.00000	0.00000	-0.00002	-0.00002	3.14158
D4	0.00000	0.00000	0.00000	0.00001	0.00001	0.00001
D5	0.00000	0.00000	0.00000	-0.00003	-0.00003	-0.00003
D6	-3.14159	0.00000	0.00000	-0.00003	-0.00003	3.14156
D7	-3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D8	0.00000	0.00000	0.00000	-0.00001	-0.00001	-0.00001
D9	0.00000	0.00000	0.00000	0.00004	0.00004	0.00004
D10	3.14159	0.00000	0.00000	0.00012	0.00012	-3.14148
D11	3.14159	0.00000	0.00000	0.00001	0.00001	-3.14158
D12	0.00000	0.00000	0.00000	0.00009	0.00009	0.00009
D13	0.00000	0.00000	0.00000	-0.00007	-0.00007	-0.00007
D14	-3.14159	0.00000	0.00000	-0.00010	-0.00010	3.14150
D15	-3.14159	0.00000	0.00000	-0.00015	-0.00015	3.14145
D16	0.00001	0.00000	0.00000	-0.00018	-0.00018	-0.00017
D17	-3.14159	0.00000	0.00000	-0.00011	-0.00011	3.14149
D18	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D19	0.00000	0.00000	0.00000	-0.00003	-0.00003	-0.00003
D20	3.14159	0.00000	0.00000	0.00008	0.00008	-3.14152
D21	0.00000	0.00000	0.00000	0.00005	0.00005	0.00005
D22	3.14159	0.00000	0.00000	0.00010	0.00010	-3.14149
D23	3.14159	0.00000	0.00000	0.00008	0.00008	-3.14151
D24	0.00000	0.00000	0.00000	0.00014	0.00014	0.00013
D25	-0.00001	0.00001	0.00000	0.00035	0.00035	0.00034
D26	3.14158	0.00001	0.00000	0.00037	0.00037	-3.14124
D27	3.14158	0.00001	0.00000	0.00031	0.00031	-3.14129

This journal is © The Royal Society of Chemistry 2014

D28	-0.00001	0.00001	0.00000	0.00033	0.00033	0.00032
D29	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D30	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D31	-3.14159	0.00000	0.00000	-0.00005	-0.00005	3.14154
D32	0.00000	0.00000	0.00000	-0.00005	-0.00005	-0.00005
D33	0.00000	0.00000	0.00000	0.00007	0.00007	0.00007
D34	3.14159	0.00000	0.00000	0.00009	0.00009	-3.14151
D35	-3.14159	0.00000	0.00000	-0.00004	-0.00004	3.14156
D36	0.00000	0.00000	0.00000	-0.00002	-0.00002	-0.00002
D37	0.00001	-0.00001	0.00000	-0.00031	-0.00031	-0.00030
D38	-3.14159	0.00000	0.00000	-0.00024	-0.00024	3.14136
D39	-3.14158	-0.00001	0.00000	-0.00033	-0.00033	3.14127
D40	0.00001	0.00000	0.00000	-0.00026	-0.00026	-0.00025
D41	0.00138	-0.00010	0.00042	-0.05034	-0.04986	-0.04848
D42	3.14011	0.00010	-0.00046	0.05347	0.05296	-3.09012
D43	-3.14021	-0.00010	0.00042	-0.05032	-0.04984	3.09314
D44	-0.00149	0.00010	-0.00046	0.05349	0.05298	0.05149
D45	0.00000	0.00000	0.00000	0.00010	0.00010	0.00010
D46	3.14159	0.00000	0.00000	0.00008	0.00008	-3.14151
D47	3.14159	0.00000	0.00000	0.00003	0.00003	-3.14156
D48	0.00000	0.00000	0.00000	0.00001	0.00001	0.00001
D49	-3.14159	0.00000	0.00000	-0.00007	-0.00007	3.14152
D50	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D51	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D52	3.14159	0.00000	0.00000	0.00007	0.00007	-3.14153
D53	0.00000	0.00000	0.00000	-0.00003	-0.00003	-0.00003

```
   D54       -3.14159   0.00000   0.00000  -0.00004  -0.00004
3.14156
   D55       -3.14159   0.00000   0.00000  -0.00001  -0.00001
3.14158
   D56        0.00000   0.00000   0.00000  -0.00002  -0.00002  -
0.00002
   D57        0.00000   0.00000   0.00000   0.00001   0.00001
0.00000
   D58       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D59        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D60        0.00000   0.00000   0.00000  -0.00001  -0.00001  -
0.00001
   D61        0.00000   0.00000   0.00000   0.00001   0.00001
0.00001
   D62       -3.14159   0.00000   0.00000  -0.00003  -0.00002
3.14157
   D63        3.14159   0.00000   0.00000   0.00002   0.00002  -
3.14157
   D64        0.00000   0.00000   0.00000  -0.00002  -0.00002  -
0.00002
   D65        0.00000   0.00000   0.00000  -0.00001  -0.00001  -
0.00001
   D66       -3.14159   0.00000   0.00000  -0.00008  -0.00008
3.14151
   D67        3.14159   0.00000   0.00000   0.00002   0.00002  -
3.14157
   D68        0.00000   0.00000   0.00000  -0.00005  -0.00005  -
0.00005
         Item               Value     Threshold  Converged?
 Maximum Force            0.001680     0.000450     NO
 RMS     Force            0.000359     0.000300     NO
 Maximum Displacement     0.063541     0.001800     NO
 RMS     Displacement     0.009722     0.001200     NO
 Predicted change in Energy=-5.093401D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -6.633888   -4.463775    0.010908
    2          6             0       -5.266119   -4.409116    0.013558
    3          6             0       -4.575974   -3.155470    0.015171
    4          6             0       -5.315885   -1.911020    0.014073
    5          6             0       -6.747051   -2.027787    0.011249
    6          6             0       -7.375068   -3.250175    0.009740
    7          6             0       -3.179280   -3.124466    0.017732
```

8	6	0	-4.596849	-0.671075	0.015859
9	6	0	-3.165685	-0.667726	0.018273
10	6	0	-2.457100	-1.927869	0.019265
11	6	0	-1.027078	-1.949040	0.021771
12	1	0	-0.526505	-2.914785	0.022466
13	6	0	-0.306928	-0.783621	0.023249
14	6	0	-0.994594	0.460741	0.022276
15	6	0	-2.368944	0.523685	0.019893
16	1	0	-2.634240	-4.067238	0.018465
17	1	0	-7.152905	-5.418167	0.009678
18	1	0	-4.671863	-5.320136	0.014474
19	1	0	-7.372874	-1.145209	0.010182
20	1	0	-8.461486	-3.287506	0.007607
21	1	0	0.779642	-0.804338	0.025155
22	1	0	-0.421759	1.384842	0.023474
23	1	0	-2.866340	1.482145	0.019274
24	6	0	-5.375853	0.586156	0.015153
25	1	0	-6.469877	0.460802	-0.035055
26	8	0	-4.940384	1.730780	-0.033703

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.368863	0.000000			
3	C	2.438583	1.431059	0.000000		
4	C	2.872926	2.498591	1.447800	0.000000	
5	C	2.438615	2.804263	2.446479	1.435925	0.000000
6	C	1.422032	2.406412	2.800700	2.456337	1.374278
7	C	3.705147	2.450560	1.397041	2.457141	3.732524
8	C	4.305128	3.797483	2.484483	1.433345	2.542452
9	C	5.141836	4.290669	2.859685	2.483778	3.830927
10	C	4.886353	3.747960	2.448806	2.858839	4.291122
11	C	6.144943	4.901174	3.748357	4.288982	5.720524
12	H	6.300764	4.969613	4.056623	4.893442	6.283478
13	C	7.319434	6.143117	4.883697	5.134273	6.559213
14	C	7.486830	6.477770	5.089530	4.929388	6.267668
15	C	6.562361	5.720680	4.290360	3.822601	5.067337
16	H	4.019264	2.653996	2.145149	3.441005	4.590711
17	H	1.086391	2.139664	3.429344	3.959135	3.414586
18	H	2.140772	1.087704	2.166789	3.469415	3.891783
19	H	3.399850	3.884780	3.444390	2.194923	1.081942
20	H	2.173416	3.386505	3.887762	3.433594	2.127485
21	H	8.267533	7.038876	5.848978	6.195184	7.625492
22	H	8.532117	7.552342	6.154024	5.900446	7.187176
23	H	7.039066	6.361283	4.942706	4.184957	5.232553
24	C	5.204275	4.996477	3.826170	2.497896	2.951762
25	H	4.927522	5.016721	4.082500	2.638115	2.504405
26	O	6.422029	6.148712	4.900064	3.661419	4.170479

		6	7	8	9	10
6	C	0.000000				
7	C	4.197678	0.000000			
8	C	3.790817	2.833484	0.000000		

This journal is © The Royal Society of Chemistry 2014

9	C	4.938423	2.456778	1.431169	0.000000	
10	C	5.092641	1.397637	2.481545	1.445703	0.000000
11	C	6.479974	2.452267	3.791634	2.493074	1.430180
12	H	6.856782	2.661053	4.647793	3.466204	2.168228
13	C	7.486165	3.705400	4.291403	2.861110	2.435685
14	C	7.381158	4.198402	3.775882	2.446853	2.800784
15	C	6.269242	3.737064	2.528048	1.433268	2.453138
16	H	4.810729	1.088986	3.922469	3.440802	2.146691
17	H	2.179345	4.588119	5.391507	6.201991	5.850886
18	H	3.404714	2.654955	4.649667	4.890144	4.051256
19	H	2.104967	4.637213	2.816230	4.234205	4.977698
20	H	1.087062	5.284732	4.667034	5.908373	6.156412
21	H	8.513615	4.588693	5.378149	3.947697	3.426200
22	H	8.356559	5.285623	4.653840	3.426688	3.888018
23	H	6.536327	4.617228	2.762432	2.170611	3.434483
24	C	4.326006	4.312036	1.479013	2.541077	3.852202
25	H	3.820043	4.866719	2.189057	3.492005	4.670233
26	O	5.544320	5.165031	2.426805	2.984139	4.422129

		11	12	13	14	15
11	C	0.000000				
12	H	1.087768	0.000000			
13	C	1.369971	2.142447	0.000000		
14	C	2.410000	3.407827	1.421731	0.000000	
15	C	2.813356	3.900983	2.441509	1.375793	0.000000
16	H	2.658899	2.402231	4.024742	4.815709	4.598582
17	H	7.039940	7.083521	8.267201	8.513902	7.628368
18	H	4.964756	4.792680	6.295452	6.851344	6.281219
19	H	6.396514	7.071373	7.075204	6.577361	5.274904
20	H	7.553947	7.943745	8.530329	8.354882	7.186404
21	H	2.138829	2.481937	1.086769	2.179070	3.417201
22	H	3.388390	4.300903	2.171501	1.087246	2.129116
23	H	3.893060	4.980747	3.418230	2.132301	1.079838
24	C	5.033796	5.981039	5.250748	4.383060	3.007562
25	H	5.952698	6.835318	6.287601	5.475583	4.101783
26	O	5.371975	6.408336	5.272037	4.145527	2.841172

		16	17	18	19	20
16	H	0.000000				
17	H	4.716293	0.000000			
18	H	2.392003	2.482983	0.000000		
19	H	5.567133	4.278617	4.972474	0.000000	
20	H	5.879192	2.500421	4.300334	2.403023	0.000000
21	H	4.722409	9.176762	7.078944	8.159652	9.568954
22	H	5.883900	9.570238	7.938527	7.397251	9.298833
23	H	5.554235	8.123364	7.037824	5.216504	7.352236
24	C	5.400976	6.261777	5.948100	2.643055	4.952418
25	H	5.934486	5.918683	6.054300	1.843019	4.244778
26	O	6.240036	7.483621	7.056192	3.766994	6.130503

		21	22	23	24	25
21	H	0.000000				
22	H	2.497174	0.000000			
23	H	4.303629	2.446520	0.000000		
24	C	6.310601	5.018069	2.664671	0.000000	

```
   25  H    7.359329   6.118578   3.745874   1.102326   0.000000
   26  O    6.256915   4.532208   2.089566   1.225636   1.988013
                  26
   26  O    0.000000
 Stoichiometry    C15H10O
 Framework group  C1[X(C15H10O)]
 Deg. of freedom    72
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        3.783336   -0.995554    0.003162
    2          6             0        2.613866   -1.706974    0.005822
    3          6             0        1.345250   -1.044761    0.001756
    4          6             0        1.272822    0.401209   -0.005353
    5          6             0        2.529469    1.095985   -0.007836
    6          6             0        3.729039    0.425423   -0.003753
    7          6             0        0.164779   -1.791890    0.004720
    8          6             0       -0.012275    1.036022   -0.009419
    9          6             0       -1.206151    0.246785   -0.006051
   10          6             0       -1.098948   -1.194920    0.001103
   11          6             0       -2.278302   -2.003948    0.004476
   12          1             0       -2.160771   -3.085334    0.009851
   13          6             0       -3.523084   -1.431822    0.001035
   14          6             0       -3.638977   -0.014839   -0.005986
   15          6             0       -2.529109    0.798172   -0.009432
   16          1             0        0.232561   -2.878750    0.010142
   17          1             0        4.743807   -1.503227    0.006286
   18          1             0        2.623084   -2.794626    0.011126
   19          1             0        2.562284    2.177418   -0.012999
   20          1             0        4.654582    0.995573   -0.005863
   21          1             0       -4.416627   -2.050402    0.003616
   22          1             0       -4.627509    0.437822   -0.008733
   23          1             0       -2.645256    1.871731   -0.014840
   24          6             0       -0.059215    2.514270   -0.017131
   25          1             0        0.921426    3.015588    0.029171
   26          8             0       -1.055323    3.226908    0.028695
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9691135      0.4403663
0.3027905
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   324 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   324 basis functions,   552 primitive gaussians,   324 cartesian
basis functions
    54 alpha electrons       54 beta electrons
```

```
      nuclear repulsion energy       963.2161484381 Hartrees.
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   324 RedAO= T  NBF=   324
 NBsUse=   317 1.00D-06 NBFU=   317
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Restarting incremental Fock formation.
 SCF Done:  E(RB+HF-LYP) =  -652.867691703     A.U. after   20 cycles
             Convg  =    0.5877D-08             -V/T =  2.0097
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
```

This journal is © The Royal Society of Chemistry 2014

Number	Number	X	Y	Z
1	6	-0.000072115	0.000126954	0.000028514
2	6	0.000291881	0.000061443	-0.000024116
3	6	-0.000445906	0.000499804	-0.000242946
4	6	0.000398693	-0.000717363	0.000310733
5	6	-0.000016166	0.000167829	0.000085201
6	6	-0.000071295	-0.000037500	-0.000003053
7	6	0.000237951	-0.000333849	0.000038715
8	6	-0.000044073	-0.000048094	0.002982947
9	6	0.000232953	0.000213428	0.000174775
10	6	-0.000120477	0.000443850	-0.000170518
11	6	-0.000250986	-0.000279108	-0.000018155
12	1	0.000040747	0.000057735	-0.000008334
13	6	0.000059633	0.000288075	-0.000005442
14	6	0.000363336	-0.000107717	0.000018412
15	6	-0.000382638	-0.000427956	0.000226080
16	1	-0.000032552	0.000091600	0.000043167
17	1	0.000030347	-0.000041011	-0.000002730
18	1	-0.000119741	-0.000043292	-0.000013128
19	1	0.000049314	0.000038380	0.000123270
20	1	0.000031310	-0.000031455	-0.000008736
21	1	-0.000010631	-0.000042312	-0.000004822
22	1	-0.000076046	0.000008258	-0.000002469
23	1	-0.000174137	0.000148070	-0.000059951
24	6	-0.000286415	-0.000459134	-0.011035793
25	1	0.000036365	0.000067023	0.003643390
26	8	0.000330649	0.000356345	0.003924987

Cartesian Forces: Max   0.011035793 RMS   0.001444488

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal Forces: Max   0.003626369 RMS   0.000601211
 Search for a local minimum.
 Step number   6 out of a maximum of 152
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points 2 3 4 6 5

 Trust test=-6.09D+00 RLast= 1.12D-01 DXMaxT set to 3.00D-01
 Energy Rises -- skip Quadratic search.
 Quartic linear search produced a step of -0.87560.
 Iteration 1 RMS(Cart)= 0.00850764 RMS(Int)= 0.00021607
 Iteration 2 RMS(Cart)= 0.00022069 RMS(Int)= 0.00002256
 Iteration 3 RMS(Cart)= 0.00000013 RMS(Int)= 0.00002256
 Variable   Old X   -DE/DX   Delta X   Delta X   Delta X   New
X
                                 (Linear)   (Quad)   (Total)
    R1   2.58678   0.00008   0.00021   0.00000   0.00021
2.58698

This journal is © The Royal Society of Chemistry 2014

R2	2.68725	-0.00004	0.00083	0.00000	0.00083
2.68808					
R3	2.05298	0.00002	0.00058	0.00000	0.00058
2.05356					
R4	2.70431	-0.00008	0.00147	0.00000	0.00147
2.70578					
R5	2.05546	-0.00003	0.00071	0.00000	0.00071
2.05617					
R6	2.73595	-0.00053	0.00288	0.00000	0.00288
2.73883					
R7	2.64002	0.00012	0.00020	0.00000	0.00020
2.64022					
R8	2.71350	-0.00004	0.00109	0.00000	0.00109
2.71459					
R9	2.70863	-0.00008	0.00073	0.00000	0.00073
2.70936					
R10	2.59701	0.00000	0.00032	0.00000	0.00032
2.59733					
R11	2.04457	0.00000	0.00071	0.00000	0.00071
2.04528					
R12	2.05425	-0.00003	0.00063	0.00000	0.00063
2.05487					
R13	2.64115	0.00011	-0.00049	0.00000	-0.00049
2.64066					
R14	2.05788	-0.00010	0.00105	0.00000	0.00105
2.05893					
R15	2.70452	-0.00008	0.00148	0.00000	0.00148
2.70600					
R16	2.79493	0.00002	-0.00255	0.00000	-0.00255
2.79238					
R17	2.73198	-0.00020	0.00167	0.00000	0.00167
2.73365					
R18	2.70848	-0.00033	0.00179	0.00000	0.00179
2.71027					
R19	2.70265	-0.00010	0.00130	0.00000	0.00130
2.70395					
R20	2.05558	-0.00003	0.00072	0.00000	0.00072
2.05630					
R21	2.58887	0.00015	0.00034	0.00000	0.00034
2.58921					
R22	2.68668	-0.00014	0.00085	0.00000	0.00085
2.68754					
R23	2.05370	-0.00001	0.00067	0.00000	0.00067
2.05437					
R24	2.59987	0.00023	-0.00055	0.00000	-0.00055
2.59932					
R25	2.05460	-0.00003	0.00071	0.00000	0.00071
2.05531					
R26	2.04060	0.00013	0.00119	0.00000	0.00119
2.04178					
R27	3.94871	-0.00015	-0.03355	0.00000	-0.03355
3.91516					

This journal is © The Royal Society of Chemistry 2014

R28	2.08309	-0.00021	0.00347	0.00000	0.00347
2.08656					
R29	2.31612	0.00026	0.00071	0.00000	0.00071
2.31683					
A1	2.07913	0.00005	-0.00050	0.00000	-0.00050
2.07862					
A2	2.10882	-0.00007	0.00042	0.00000	0.00042
2.10925					
A3	2.09523	0.00002	0.00008	0.00000	0.00008
2.09532					
A4	2.11397	-0.00005	0.00072	0.00000	0.00072
2.11469					
A5	2.10884	-0.00011	0.00064	0.00000	0.00064
2.10949					
A6	2.06037	0.00015	-0.00136	0.00000	-0.00136
2.05901					
A7	2.10194	-0.00003	-0.00041	0.00000	-0.00041
2.10153					
A8	2.09623	0.00003	0.00030	0.00000	0.00030
2.09653					
A9	2.08502	0.00000	0.00011	0.00000	0.00011
2.08513					
A10	2.02580	0.00021	-0.00085	0.00000	-0.00086
2.02495					
A11	2.07967	0.00013	-0.00090	0.00000	-0.00090
2.07877					
A12	2.17771	-0.00034	0.00176	0.00000	0.00176
2.17947					
A13	2.12680	-0.00007	0.00056	0.00000	0.00056
2.12737					
A14	2.10619	-0.00003	-0.00041	0.00000	-0.00041
2.10577					
A15	2.05020	0.00010	-0.00015	0.00000	-0.00015
2.05005					
A16	2.11872	-0.00012	0.00049	0.00000	0.00049
2.11922					
A17	2.08472	0.00003	-0.00018	0.00000	-0.00018
2.08454					
A18	2.07974	0.00009	-0.00031	0.00000	-0.00031
2.07943					
A19	2.13600	-0.00013	0.00136	0.00000	0.00136
2.13737					
A20	2.07278	0.00008	-0.00098	0.00000	-0.00098
2.07181					
A21	2.07440	0.00005	-0.00039	0.00000	-0.00039
2.07401					
A22	2.09864	0.00002	-0.00027	0.00000	-0.00027
2.09837					
A23	2.06137	0.00002	0.00221	0.00000	0.00221
2.06358					
A24	2.12318	-0.00004	-0.00194	0.00000	-0.00194
2.12124					

This journal is © The Royal Society of Chemistry 2014

A25	2.08070	-0.00010	0.00116	0.00000	0.00116
2.08186					
A26	2.16257	0.00007	-0.00278	0.00000	-0.00278
2.15979					
A27	2.03991	0.00003	0.00162	0.00000	0.00162
2.04153					
A28	2.08634	0.00009	-0.00147	0.00000	-0.00147
2.08487					
A29	2.09900	-0.00015	0.00332	0.00000	0.00332
2.10233					
A30	2.09784	0.00007	-0.00185	0.00000	-0.00185
2.09599					
A31	2.06380	0.00007	-0.00025	0.00000	-0.00025
2.06356					
A32	2.10949	-0.00002	0.00010	0.00000	0.00010
2.10960					
A33	2.10989	-0.00005	0.00015	0.00000	0.00015
2.11003					
A34	2.08323	-0.00007	0.00124	0.00000	0.00124
2.08448					
A35	2.10523	-0.00001	-0.00042	0.00000	-0.00042
2.10481					
A36	2.09472	0.00008	-0.00082	0.00000	-0.00082
2.09390					
A37	2.12142	-0.00004	-0.00039	0.00000	-0.00039
2.12103					
A38	2.08182	0.00009	-0.00075	0.00000	-0.00075
2.08107					
A39	2.07994	-0.00005	0.00115	0.00000	0.00115
2.08109					
A40	2.11447	0.00003	-0.00071	0.00000	-0.00071
2.11375					
A41	2.07346	0.00002	-0.00982	0.00000	-0.00982
2.06364					
A42	2.09526	-0.00006	0.01053	0.00000	0.01053
2.10579					
A43	2.01097	0.00033	-0.00019	0.00000	-0.00003
2.01093					
A44	2.22275	0.00021	0.00254	0.00000	0.00269
2.22544					
A45	2.04543	0.00003	0.00119	0.00000	0.00134
2.04677					
D1	0.00001	-0.00001	-0.00001	0.00000	-0.00001
0.00000					
D2	-3.14156	-0.00002	-0.00003	0.00000	-0.00003
-3.14159					
D3	3.14158	0.00001	0.00001	0.00000	0.00001
3.14159					
D4	0.00001	-0.00001	-0.00001	0.00000	-0.00001
0.00000					
D5	-0.00003	0.00002	0.00003	0.00000	0.00003
0.00000					

This journal is © The Royal Society of Chemistry 2014

D6	3.14156	0.00002	0.00003	0.00000	0.00003
3.14159					
D7	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D8	-0.00001	0.00000	0.00001	0.00000	0.00001
0.00000					
D9	0.00004	-0.00003	-0.00004	0.00000	-0.00004
0.00000					
D10	-3.14148	-0.00007	-0.00010	0.00000	-0.00010	-
3.14158					
D11	-3.14158	-0.00001	-0.00001	0.00000	-0.00001	-
3.14159					
D12	0.00009	-0.00005	-0.00008	0.00000	-0.00008
0.00001					
D13	-0.00007	0.00004	0.00006	0.00000	0.00006	-
0.00001					
D14	3.14150	0.00006	0.00009	0.00000	0.00009
3.14158					
D15	3.14145	0.00009	0.00013	0.00000	0.00013
3.14158					
D16	-0.00017	0.00010	0.00016	0.00000	0.00016	-
0.00002					
D17	3.14149	0.00007	0.00009	0.00000	0.00009
3.14158					
D18	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D19	-0.00003	0.00002	0.00003	0.00000	0.00003
0.00000					
D20	-3.14152	-0.00004	-0.00007	0.00000	-0.00007	-
3.14159					
D21	0.00005	-0.00003	-0.00004	0.00000	-0.00004
0.00000					
D22	-3.14149	-0.00007	-0.00009	0.00000	-0.00009	-
3.14158					
D23	-3.14151	-0.00005	-0.00007	0.00000	-0.00007	-
3.14158					
D24	0.00013	-0.00008	-0.00012	0.00000	-0.00012
0.00001					
D25	0.00034	-0.00021	-0.00030	0.00000	-0.00030
0.00003					
D26	-3.14124	-0.00022	-0.00032	0.00000	-0.00032	-
3.14156					
D27	-3.14129	-0.00019	-0.00027	0.00000	-0.00027	-
3.14156					
D28	0.00032	-0.00020	-0.00029	0.00000	-0.00029
0.00003					
D29	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D30	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D31	3.14154	0.00004	0.00005	0.00000	0.00005
3.14159					

This journal is © The Royal Society of Chemistry 2014

D32	-0.00005	0.00003	0.00004	0.00000	0.00004	0.00000
D33	0.00007	-0.00004	-0.00006	0.00000	-0.00006	0.00001
D34	-3.14151	-0.00005	-0.00008	0.00000	-0.00008	-3.14158
D35	3.14156	0.00002	0.00003	0.00000	0.00003	3.14159
D36	-0.00002	0.00001	0.00002	0.00000	0.00002	0.00000
D37	-0.00030	0.00019	0.00027	0.00000	0.00027	-0.00003
D38	3.14136	0.00015	0.00021	0.00000	0.00021	3.14157
D39	3.14127	0.00020	0.00029	0.00000	0.00029	3.14156
D40	-0.00025	0.00016	0.00023	0.00000	0.00023	-0.00003
D41	-0.04848	0.00343	0.04365	0.00000	0.04365	-0.00482
D42	-3.09012	-0.00361	-0.04637	0.00000	-0.04637	-3.13649
D43	3.09314	0.00342	0.04364	0.00000	0.04364	3.13677
D44	0.05149	-0.00363	-0.04639	0.00000	-0.04639	0.00510
D45	0.00010	-0.00006	-0.00009	0.00000	-0.00009	0.00001
D46	-3.14151	-0.00005	-0.00007	0.00000	-0.00007	-3.14158
D47	-3.14156	-0.00003	-0.00003	0.00000	-0.00003	-3.14159
D48	0.00001	-0.00001	-0.00001	0.00000	-0.00001	0.00000
D49	3.14152	0.00004	0.00006	0.00000	0.00006	3.14159
D50	0.00000	0.00001	0.00000	0.00000	0.00000	0.00000
D51	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D52	-3.14153	-0.00003	-0.00006	0.00000	-0.00006	-3.14159
D53	-0.00003	0.00002	0.00003	0.00000	0.00003	0.00000
D54	3.14156	0.00003	0.00003	0.00000	0.00003	3.14159
D55	3.14158	0.00001	0.00001	0.00000	0.00001	3.14159
D56	-0.00002	0.00001	0.00001	0.00000	0.00001	0.00000
D57	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

```
   D58        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D59        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D60       -0.00001   0.00001   0.00001   0.00000   0.00001
0.00000
   D61        0.00001  -0.00001  -0.00001   0.00000  -0.00001
0.00000
   D62        3.14157   0.00001   0.00002   0.00000   0.00002
3.14159
   D63       -3.14157  -0.00001  -0.00002   0.00000  -0.00002  -
3.14159
   D64       -0.00002   0.00001   0.00001   0.00000   0.00001
0.00000
   D65       -0.00001   0.00001   0.00001   0.00000   0.00001
0.00000
   D66        3.14151   0.00005   0.00007   0.00000   0.00007
3.14159
   D67       -3.14157  -0.00001  -0.00002   0.00000  -0.00002  -
3.14159
   D68       -0.00005   0.00003   0.00004   0.00000   0.00004
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.003626     0.000450     NO
 RMS     Force            0.000601     0.000300     NO
 Maximum Displacement     0.055650     0.001800     NO
 RMS     Displacement     0.008512     0.001200     NO
 Predicted change in Energy=-6.830518D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -6.635275   -4.465087    0.011112
    2          6             0       -5.267414   -4.410116    0.015794
    3          6             0       -4.576265   -3.156132    0.014896
    4          6             0       -5.316841   -1.910316    0.008972
    5          6             0       -6.748484   -2.028241    0.004229
    6          6             0       -7.376328   -3.250908    0.005265
    7          6             0       -3.179466   -3.125397    0.019731
    8          6             0       -4.596386   -0.670745    0.008228
    9          6             0       -3.164442   -0.669184    0.013244
   10          6             0       -2.455549   -1.930154    0.019093
   11          6             0       -1.024809   -1.948810    0.024168
   12          1             0       -0.522605   -2.914129    0.028505
   13          6             0       -0.306496   -0.782045    0.023582
   14          6             0       -0.994890    0.462417    0.017847
   15          6             0       -2.368993    0.524226    0.012857
```

16	1	0	-2.635264	-4.069282	0.024153
17	1	0	-7.154634	-5.419641	0.011818
18	1	0	-4.672176	-5.320932	0.020316
19	1	0	-7.374832	-1.145588	-0.000336
20	1	0	-8.463077	-3.288140	0.001525
21	1	0	0.780450	-0.801417	0.027451
22	1	0	-0.421544	1.386646	0.017399
23	1	0	-2.877517	1.477531	0.008536
24	6	0	-5.370655	0.587812	0.002197
25	1	0	-6.467940	0.465062	-0.006141
26	8	0	-4.933454	1.733202	-0.004254

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.368973	0.000000			
3	C	2.439856	1.431839	0.000000		
4	C	2.874913	2.500298	1.449326	0.000000	
5	C	2.439484	2.804823	2.447609	1.436499	0.000000
6	C	1.422470	2.406531	2.801683	2.457374	1.374448
7	C	3.706408	2.451540	1.397146	2.458640	3.733883
8	C	4.307448	3.799109	2.485478	1.433734	2.544472
9	C	5.143497	4.291511	2.859748	2.484602	3.833076
10	C	4.888359	3.749241	2.449587	2.861379	4.294081
11	C	6.148914	4.904875	3.751074	4.292232	5.724261
12	H	6.306386	4.975073	4.060900	4.898236	6.288637
13	C	7.322459	6.146029	4.885417	5.135832	6.561447
14	C	7.489612	6.480436	5.091185	4.930437	6.269562
15	C	6.564633	5.722638	4.291515	3.823195	5.069034
16	H	4.019567	2.654138	2.145091	3.442705	4.591822
17	H	1.086696	2.140270	3.430957	3.961420	3.415642
18	H	2.141569	1.088079	2.166930	3.471026	3.892703
19	H	3.400903	3.885693	3.445939	2.195500	1.082315
20	H	2.173972	3.386930	3.889076	3.434713	2.127718
21	H	8.271380	7.042692	5.851431	6.197335	7.628269
22	H	8.535413	7.555456	6.156180	5.902031	7.189701
23	H	7.031035	6.354215	4.935243	4.174663	5.222532
24	C	5.208755	4.999013	3.827315	2.498717	2.956712
25	H	4.933018	5.020867	4.085575	2.639636	2.509058
26	O	6.427691	6.152421	4.902402	3.663658	4.176465

		6	7	8	9	10
6	C	0.000000				
7	C	4.198764	0.000000			
8	C	3.792800	2.834274	0.000000		
9	C	4.940177	2.456267	1.431953	0.000000	
10	C	5.094963	1.397376	2.483830	1.446585	0.000000
11	C	6.483642	2.454979	3.793398	2.493109	1.430871
12	H	6.862031	2.665261	4.650685	3.466888	2.169001
13	C	7.488535	3.707461	4.291361	2.860193	2.436515
14	C	7.383204	4.200569	3.775569	2.446937	2.803199
15	C	6.270973	3.738537	2.527698	1.434214	2.455914
16	H	4.811214	1.089539	3.923813	3.441049	2.146670

17	H	2.180044	4.589726	5.394131	6.203907	5.853031
18	H	3.405534	2.654913	4.650820	4.889997	4.051026
19	H	2.105328	4.639088	2.818743	4.237278	4.981492
20	H	1.087393	5.286148	4.669272	5.910550	6.159126
21	H	8.516662	4.591501	5.378458	3.947134	3.427216
22	H	8.359191	5.288163	4.654272	3.427820	3.890802
23	H	6.526672	4.612834	2.751291	2.165810	3.433728
24	C	4.331109	4.311558	1.477666	2.539200	3.852049
25	H	3.825407	4.868893	2.189287	3.492848	4.673005
26	O	5.550593	5.165562	2.427495	2.983483	4.422752

		11	12	13	14	15
11	C	0.000000				
12	H	1.088149	0.000000			
13	C	1.370152	2.143014	0.000000		
14	C	2.411422	3.409433	1.422184	0.000000	
15	C	2.814759	3.902779	2.441384	1.375502	0.000000
16	H	2.662699	2.407846	4.028535	4.819458	4.601234
17	H	7.044258	7.089546	8.270697	8.517106	7.630984
18	H	4.967344	4.797051	6.297672	6.853435	6.282562
19	H	6.400668	7.076833	7.077719	6.579488	5.277014
20	H	7.557919	7.949321	8.532925	8.357079	7.188333
21	H	2.139038	2.482239	1.087126	2.179266	3.417095
22	H	3.389579	4.301977	2.171749	1.087623	2.129870
23	H	3.895201	4.983241	3.422873	2.138885	1.080465
24	C	5.032029	5.980625	5.246206	4.377590	3.002355
25	H	5.954441	6.838650	6.286458	5.473103	4.099418
26	O	5.369872	6.407367	5.266497	4.138559	2.835203

		16	17	18	19	20
16	H	0.000000				
17	H	4.716813	0.000000			
18	H	2.390743	2.484435	0.000000		
19	H	5.568849	4.279738	4.973758	0.000000	
20	H	5.879974	2.501084	4.301573	2.403083	0.000000
21	H	4.727162	9.181166	7.082175	8.162588	9.572213
22	H	5.887933	9.573927	7.941000	7.400050	9.301620
23	H	5.552123	8.115708	7.031361	5.206407	7.342353
24	C	5.401053	6.266750	5.949913	2.649794	4.958435
25	H	5.937221	5.924660	6.058316	1.848427	4.250548
26	O	6.241098	7.489797	7.059014	3.774622	6.137764

		21	22	23	24	25
21	H	0.000000				
22	H	2.496499	0.000000			
23	H	4.309836	2.457670	0.000000		
24	C	6.306084	5.013190	2.647145	0.000000	
25	H	7.358278	6.116271	3.730475	1.104160	0.000000
26	O	6.250920	4.525252	2.071813	1.226012	1.990686

		26
26	O	0.000000

Stoichiometry C15H10O
Framework group C1[X(C15H10O)]
Deg. of freedom 72
Full point group C1

This journal is © The Royal Society of Chemistry 2014

```
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        3.786500   -0.992835    0.000314
    2          6             0        2.617294   -1.704907    0.000577
    3          6             0        1.347178   -1.043873    0.000174
    4          6             0        1.273503    0.403579   -0.000531
    5          6             0        2.530685    1.098578   -0.000777
    6          6             0        3.730750    0.428542   -0.000372
    7          6             0        0.167307   -1.792153    0.000468
    8          6             0       -0.013027    1.036377   -0.000933
    9          6             0       -1.205991    0.244338   -0.000599
   10          6             0       -1.097545   -1.198177    0.000110
   11          6             0       -2.278307   -2.006380    0.000443
   12          1             0       -2.161587   -3.088250    0.000975
   13          6             0       -3.522717   -1.433006    0.000101
   14          6             0       -3.639083   -0.015591   -0.000594
   15          6             0       -2.529379    0.797159   -0.000935
   16          1             0        0.237189   -2.879449    0.001005
   17          1             0        4.747710   -1.499768    0.000623
   18          1             0        2.626366   -2.792948    0.001103
   19          1             0        2.563115    2.180408   -0.001288
   20          1             0        4.656101    0.999637   -0.000581
   21          1             0       -4.416872   -2.051333    0.000356
   22          1             0       -4.628437    0.436186   -0.000866
   23          1             0       -2.634181    1.872529   -0.001469
   24          6             0       -0.065710    2.513103   -0.001696
   25          1             0        0.915797    3.018863    0.002918
   26          8             0       -1.064244    3.224450    0.002840
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9693176      0.4399500
0.3026050
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   324 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   324 basis functions,   552 primitive gaussians,   324 cartesian
basis functions
    54 alpha electrons       54 beta electrons
       nuclear repulsion energy       962.9688474162 Hartrees.
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   324 RedAO= T  NBF=   324
 NBsUse=   317 1.00D-06 NBFU=   317
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
```

```
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -652.868008115     A.U. after   12 cycles
             Convg  =    0.7857D-08             -V/T =  2.0098
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000108057    0.000395836    0.000001395
    2          6           0.000781512    0.000291260   -0.000000452
    3          6          -0.001242689    0.001095412   -0.000031229
    4          6           0.000628519   -0.001521560    0.000037085
    5          6           0.000296788    0.000500711    0.000008025
    6          6          -0.000069351   -0.000187151   -0.000000069
    7          6           0.000562231   -0.001087324    0.000008647
```

8	6	0.000904322	-0.000617363	0.000300801
9	6	0.000503169	-0.000021102	0.000019288
10	6	-0.000246386	0.001685396	-0.000022268
11	6	-0.000644629	-0.000582004	-0.000002473
12	1	-0.000042360	0.000293464	-0.000001766
13	6	0.000081351	0.000305507	-0.000001132
14	6	0.000576419	0.000186193	0.000003239
15	6	-0.001692394	-0.001350515	0.000020908
16	1	-0.000181229	0.000367595	0.000002684
17	1	0.000153589	0.000152852	-0.000000129
18	1	-0.000333158	0.000108397	-0.000002759
19	1	0.000203094	-0.000064937	0.000012977
20	1	0.000258111	-0.000024412	0.000000111
21	1	-0.000256360	-0.000054137	-0.000001215
22	1	-0.000251468	-0.000169755	-0.000000635
23	1	0.001195324	0.000271278	-0.000002641
24	6	-0.002118048	0.000234673	-0.001110121
25	1	0.001219111	0.000198143	0.000369362
26	8	-0.000177412	-0.000406455	0.000392370

Cartesian Forces: Max 0.002118048 RMS 0.000604899

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Internal Forces: Max 0.001538240 RMS 0.000327895
Search for a local minimum.
Step number 7 out of a maximum of 152
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points 2 3 4 6 5
7

Eigenvalues --- 0.00237 0.01524 0.02056 0.02070
0.02082
Eigenvalues --- 0.02085 0.02086 0.02088 0.02092
0.02096
Eigenvalues --- 0.02229 0.02231 0.02253 0.02258
0.02348
Eigenvalues --- 0.02350 0.02374 0.02382 0.02394
0.02425
Eigenvalues --- 0.02430 0.02501 0.02504 0.06241
0.09741
Eigenvalues --- 0.15977 0.16000 0.16000 0.16000
0.16000
Eigenvalues --- 0.16002 0.16008 0.16290 0.16486
0.19796
Eigenvalues --- 0.21983 0.22125 0.22546 0.22678
0.23175
Eigenvalues --- 0.24353 0.24714 0.24960 0.26785
0.30624
Eigenvalues --- 0.32149 0.36856 0.37230 0.37230
0.37230

```
     Eigenvalues ---    0.37230   0.37230   0.37234   0.37370
0.37585
     Eigenvalues ---    0.38074   0.40441   0.42253   0.42976
0.43421
     Eigenvalues ---    0.43637   0.44784   0.45335   0.45433
0.45642
     Eigenvalues ---    0.46115   0.51573   0.51581   0.52720
0.55500
     Eigenvalues ---    0.56173
0.816421000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-1.54655593D-04.
 Quartic linear search produced a step of -0.00201.
 Iteration  1 RMS(Cart)=  0.00516424 RMS(Int)=  0.00002942
 Iteration  2 RMS(Cart)=  0.00003674 RMS(Int)=  0.00000770
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000770
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58698  -0.00008   0.00000   0.00009   0.00009
2.58707
    R2        2.68808  -0.00038   0.00000  -0.00228  -0.00228
2.68580
    R3        2.05356  -0.00021   0.00000  -0.00127  -0.00127
2.05229
```

This journal is © The Royal Society of Chemistry 2014

R4	2.70578	-0.00072	0.00000	-0.00449	-0.00449
2.70129					
R5	2.05617	-0.00028	0.00000	-0.00193	-0.00193
2.05424					
R6	2.73883	-0.00154	0.00000	-0.01052	-0.01052
2.72831					
R7	2.64022	0.00000	0.00000	0.00019	0.00020
2.64042					
R8	2.71459	-0.00070	0.00000	-0.00330	-0.00330
2.71129					
R9	2.70936	-0.00072	0.00000	-0.00299	-0.00299
2.70637					
R10	2.59733	-0.00026	0.00000	-0.00069	-0.00069
2.59664					
R11	2.04528	-0.00017	0.00000	-0.00181	-0.00181
2.04347					
R12	2.05487	-0.00026	0.00000	-0.00172	-0.00172
2.05315					
R13	2.64066	0.00020	0.00000	0.00181	0.00182
2.64247					
R14	2.05893	-0.00041	0.00000	-0.00329	-0.00329
2.05564					
R15	2.70600	-0.00082	0.00000	-0.00510	-0.00511
2.70089					
R16	2.79238	0.00032	0.00000	0.00417	0.00416
2.79654					
R17	2.73365	-0.00100	0.00000	-0.00671	-0.00671
2.72694					
R18	2.71027	-0.00099	0.00000	-0.00669	-0.00670
2.70357					
R19	2.70395	-0.00068	0.00000	-0.00416	-0.00415
2.69980					
R20	2.05630	-0.00028	0.00000	-0.00195	-0.00195
2.05436					
R21	2.58921	-0.00008	0.00000	0.00045	0.00045
2.58966					
R22	2.68754	-0.00038	0.00000	-0.00197	-0.00197
2.68557					
R23	2.05437	-0.00025	0.00000	-0.00167	-0.00167
2.05270					
R24	2.59932	0.00014	0.00000	0.00207	0.00207
2.60139					
R25	2.05531	-0.00028	0.00000	-0.00194	-0.00194
2.05337					
R26	2.04178	-0.00008	0.00000	0.00015	0.00015
2.04194					
R27	3.91516	0.00043	-0.00001	0.01976	0.01976
3.93492					
R28	2.08656	-0.00124	0.00000	-0.01180	-0.01180
2.07476					
R29	2.31683	-0.00034	0.00000	-0.00233	-0.00233
2.31450					

This journal is © The Royal Society of Chemistry 2014

A1	2.07862	0.00013	0.00000	0.00306	0.00305
2.08167					
A2	2.10925	-0.00013	0.00000	-0.00274	-0.00274
2.10651					
A3	2.09532	-0.00001	0.00000	-0.00032	-0.00032
2.09500					
A4	2.11469	-0.00020	0.00000	-0.00251	-0.00251
2.11218					
A5	2.10949	-0.00013	0.00000	-0.00398	-0.00398
2.10551					
A6	2.05901	0.00033	0.00000	0.00649	0.00649
2.06550					
A7	2.10153	0.00002	0.00000	-0.00023	-0.00023
2.10130					
A8	2.09653	0.00000	0.00000	-0.00036	-0.00036
2.09616					
A9	2.08513	-0.00002	0.00000	0.00059	0.00059
2.08572					
A10	2.02495	0.00056	0.00000	0.00514	0.00515
2.03010					
A11	2.07877	0.00029	0.00000	0.00265	0.00265
2.08142					
A12	2.17947	-0.00085	0.00000	-0.00779	-0.00779
2.17167					
A13	2.12737	-0.00025	0.00000	-0.00250	-0.00249
2.12487					
A14	2.10577	-0.00001	0.00000	-0.00037	-0.00037
2.10540					
A15	2.05005	0.00026	0.00000	0.00287	0.00287
2.05291					
A16	2.11922	-0.00026	0.00000	-0.00297	-0.00297
2.11625					
A17	2.08454	0.00010	0.00000	0.00036	0.00036
2.08490					
A18	2.07943	0.00016	0.00000	0.00261	0.00261
2.08204					
A19	2.13737	-0.00047	0.00000	-0.00549	-0.00549
2.13188					
A20	2.07181	0.00026	0.00000	0.00320	0.00320
2.07501					
A21	2.07401	0.00021	0.00000	0.00229	0.00229
2.07630					
A22	2.09837	0.00017	0.00000	0.00046	0.00047
2.09884					
A23	2.06358	-0.00034	0.00000	-0.00156	-0.00154
2.06203					
A24	2.12124	0.00017	0.00000	0.00110	0.00107
2.12231					
A25	2.08186	-0.00022	0.00000	-0.00277	-0.00276
2.07910					
A26	2.15979	0.00016	0.00000	0.00345	0.00343
2.16322					

This journal is © The Royal Society of Chemistry 2014

```
   A27        2.04153   0.00005   0.00000  -0.00068  -0.00067
2.04086
   A28        2.08487   0.00025   0.00000   0.00455   0.00455
2.08942
   A29        2.10233  -0.00054   0.00000  -0.00764  -0.00763
2.09469
   A30        2.09599   0.00030   0.00000   0.00309   0.00309
2.09908
   A31        2.06356   0.00015   0.00000   0.00265   0.00265
2.06620
   A32        2.10960  -0.00010   0.00000  -0.00087  -0.00087
2.10872
   A33        2.11003  -0.00005   0.00000  -0.00177  -0.00177
2.10826
   A34        2.08448  -0.00017   0.00000  -0.00162  -0.00162
2.08285
   A35        2.10481   0.00002   0.00000  -0.00065  -0.00065
2.10416
   A36        2.09390   0.00015   0.00000   0.00228   0.00228
2.09617
   A37        2.12103  -0.00011   0.00000  -0.00084  -0.00084
2.12018
   A38        2.08107   0.00018   0.00000   0.00282   0.00282
2.08389
   A39        2.08109  -0.00007   0.00000  -0.00198  -0.00197
2.07911
   A40        2.11375   0.00002   0.00000   0.00093   0.00092
2.11468
   A41        2.06364   0.00084   0.00000   0.01496   0.01495
2.07859
   A42        2.10579  -0.00086   0.00000  -0.01589  -0.01588
2.08992
   A43        2.01093   0.00040   0.00000   0.00795   0.00791
2.01885
   A44        2.22544  -0.00066   0.00000  -0.00849  -0.00854
2.21690
   A45        2.04677   0.00027   0.00000   0.00068   0.00064
2.04741
    D1        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D2       -3.14159   0.00000   0.00000  -0.00001  -0.00001
3.14159
    D3        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
    D4        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D5        0.00000   0.00000   0.00000   0.00001   0.00001
0.00000
    D6        3.14159   0.00000   0.00000   0.00001   0.00001  -
3.14159
    D7        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
```

D8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D9	0.00000	0.00000	0.00000	-0.00001	-0.00001	0.00000
D10	-3.14158	-0.00001	0.00000	-0.00002	-0.00002	3.14159
D11	-3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D12	0.00001	-0.00001	0.00000	-0.00001	-0.00001	-0.00001
D13	-0.00001	0.00000	0.00000	0.00001	0.00001	0.00001
D14	3.14158	0.00001	0.00000	0.00001	0.00001	-3.14159
D15	3.14158	0.00001	0.00000	0.00002	0.00002	-3.14158
D16	-0.00002	0.00001	0.00000	0.00002	0.00002	0.00001
D17	3.14158	0.00001	0.00000	0.00001	0.00001	-3.14159
D18	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D19	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D20	-3.14159	0.00000	0.00000	-0.00001	-0.00001	3.14159
D21	0.00000	0.00000	0.00000	-0.00001	-0.00001	-0.00001
D22	-3.14158	-0.00001	0.00000	-0.00002	-0.00002	3.14158
D23	-3.14158	0.00000	0.00000	-0.00001	-0.00001	3.14159
D24	0.00001	-0.00001	0.00000	-0.00002	-0.00002	-0.00001
D25	0.00003	-0.00002	0.00000	-0.00005	-0.00005	-0.00001
D26	-3.14156	-0.00002	0.00000	-0.00005	-0.00005	3.14158
D27	-3.14156	-0.00002	0.00000	-0.00005	-0.00005	3.14158
D28	0.00003	-0.00002	0.00000	-0.00005	-0.00005	-0.00002
D29	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D30	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D31	3.14159	0.00000	0.00000	0.00001	0.00001	-3.14159
D32	0.00000	0.00000	0.00000	0.00001	0.00001	0.00000
D33	0.00001	0.00000	0.00000	-0.00001	-0.00001	0.00000

D34	-3.14158	-0.00001	0.00000	-0.00001	-0.00001
3.14159					
D35	3.14159	0.00000	0.00000	0.00001	0.00001
-3.14159					
D36	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D37	-0.00003	0.00002	0.00000	0.00004	0.00004
0.00001					
D38	3.14157	0.00001	0.00000	0.00002	0.00002
-3.14159					
D39	3.14156	0.00002	0.00000	0.00004	0.00004
-3.14158					
D40	-0.00003	0.00001	0.00000	0.00003	0.00003
0.00000					
D41	-0.00482	0.00034	0.00001	0.00867	0.00868
0.00386					
D42	-3.13649	-0.00036	-0.00001	-0.00949	-0.00951
3.13719					
D43	3.13677	0.00034	0.00001	0.00867	0.00868
-3.13773					
D44	0.00510	-0.00036	-0.00001	-0.00950	-0.00951
-0.00441					
D45	0.00001	-0.00001	0.00000	-0.00001	-0.00001
0.00000					
D46	-3.14158	0.00000	0.00000	-0.00001	-0.00001
3.14159					
D47	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D48	0.00000	0.00000	0.00000	0.00000	0.00000
0.00001					
D49	3.14159	0.00000	0.00000	0.00001	0.00001
-3.14159					
D50	0.00000	0.00000	0.00000	0.00000	0.00000
-0.00001					
D51	0.00000	0.00000	0.00000	0.00000	0.00000
-0.00001					
D52	-3.14159	0.00000	0.00000	-0.00002	-0.00002
3.14158					
D53	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D54	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D55	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D56	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D57	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D58	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D59	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					

```
   D60        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D61        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D62        3.14159   0.00000   0.00000   0.00001   0.00001  -
3.14159
   D63       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D64        0.00000   0.00000   0.00000   0.00001   0.00001
0.00000
   D65        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D66        3.14159   0.00001   0.00000   0.00002   0.00002  -
3.14158
   D67       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D68        0.00000   0.00000   0.00000   0.00001   0.00001
0.00001
         Item               Value     Threshold  Converged?
 Maximum Force            0.001538     0.000450     NO
 RMS     Force            0.000328     0.000300     NO
 Maximum Displacement     0.020552     0.001800     NO
 RMS     Displacement     0.005173     0.001200     NO
 Predicted change in Energy=-7.756038D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -6.632454   -4.459845    0.011146
    2          6             0       -5.264413   -4.408324    0.016257
    3          6             0       -4.574393   -3.156434    0.014855
    4          6             0       -5.312387   -1.915562    0.007976
    5          6             0       -6.742854   -2.026286    0.002820
    6          6             0       -7.373515   -3.247092    0.004351
    7          6             0       -3.177480   -3.126219    0.020156
    8          6             0       -4.596270   -0.675309    0.006708
    9          6             0       -3.167046   -0.668998    0.012218
   10          6             0       -2.459187   -1.926469    0.019038
   11          6             0       -1.030699   -1.948696    0.024633
   12          1             0       -0.528853   -2.913036    0.029705
   13          6             0       -0.310337   -0.782914    0.023630
   14          6             0       -0.998192    0.460650    0.016926
   15          6             0       -2.373436    0.521380    0.011413
   16          1             0       -2.631490   -4.067055    0.025324
   17          1             0       -7.151291   -5.413918    0.012243
   18          1             0       -4.675664   -5.322132    0.021497
   19          1             0       -7.363956   -1.141107   -0.002444
```

20	1	0	-8.459347	-3.284474	0.000286
21	1	0	0.775676	-0.804768	0.027900
22	1	0	-0.427967	1.385605	0.016119
23	1	0	-2.867585	1.482302	0.006367
24	6	0	-5.377227	0.581696	-0.000406
25	1	0	-6.468761	0.463497	-0.000424
26	8	0	-4.935756	1.724140	0.001890

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.369021	0.000000			
3	C	2.436085	1.429461	0.000000		
4	C	2.866351	2.493238	1.443761	0.000000	
5	C	2.436076	2.803583	2.445322	1.434755	0.000000
6	C	1.421263	2.407678	2.800609	2.453821	1.374082
7	C	3.703442	2.449305	1.397250	2.454316	3.731226
8	C	4.297532	3.792349	2.481234	1.432149	2.536332
9	C	5.136106	4.287369	2.857966	2.481215	3.824752
10	C	4.882030	3.745518	2.446820	2.853242	4.284860
11	C	6.138869	4.896343	3.743861	4.281848	5.712724
12	H	6.296579	4.966044	4.052883	4.886474	6.277010
13	C	7.313627	6.138935	4.880148	5.128707	6.551617
14	C	7.480389	6.473604	5.086503	4.925316	6.259888
15	C	6.553765	5.714871	4.286086	3.817870	5.057914
16	H	4.020224	2.654963	2.145744	3.437504	4.590050
17	H	1.086024	2.138117	3.425879	3.952225	3.412178
18	H	2.138380	1.087059	2.168075	3.465591	3.890530
19	H	3.398427	3.883702	3.441439	2.192903	1.081359
20	H	2.172361	3.386872	3.887090	3.431813	2.128236
21	H	8.260766	7.033379	5.844120	6.188600	7.617154
22	H	8.524375	7.547239	6.150038	5.895364	7.177672
23	H	7.034442	6.359588	4.942786	4.185993	5.227611
24	C	5.195466	4.991323	3.823400	2.498113	2.943895
25	H	4.926077	5.018504	4.085678	2.645221	2.504828
26	O	6.412531	6.141282	4.893951	3.659142	4.163089

		6	7	8	9	10
6	C	0.000000				
7	C	4.197805	0.000000			
8	C	3.785124	2.831979	0.000000		
9	C	4.933661	2.457257	1.429248	0.000000	
10	C	5.088701	1.398337	2.476423	1.443033	0.000000
11	C	6.474377	2.448520	3.786176	2.490334	1.428672
12	H	6.852856	2.657210	4.642394	3.463535	2.167860
13	C	7.480711	3.702918	4.287316	2.859002	2.434193
14	C	7.375110	4.197016	3.773151	2.445415	2.798723
15	C	6.261168	3.735176	2.524496	1.430670	2.449362
16	H	4.812440	1.087798	3.919776	3.440027	2.147519
17	H	2.178206	4.585281	5.383547	6.195844	5.846211
18	H	3.403599	2.658306	4.647524	4.891593	4.055035
19	H	2.106018	4.633331	2.806624	4.223406	4.967294
20	H	1.086483	5.284274	4.661668	5.903330	6.151946

This journal is © The Royal Society of Chemistry 2014

```
   21  H    8.507339   4.584391   5.373547   3.945090   3.423833
   22  H    8.348811   5.283597   4.649968   3.424027   3.885318
   23  H    6.532272   4.618949   2.764713   2.172050   3.433172
   24  C    4.317963   4.311374   1.479867   2.539546   3.847886
   25  H    3.819303   4.870217   2.191610   3.490562   4.667869
   26  O    5.536771   5.159249   2.423352   2.975827   4.411421
                 11         12         13         14         15
   11  C    0.000000
   12  H    1.087118   0.000000
   13  C    1.370391   2.141310   0.000000
   14  C    2.409578   3.406201   1.421141   0.000000
   15  C    2.811475   3.898465   2.440841   1.376595   0.000000
   16  H    2.655179   2.398512   4.021609   4.813299   4.595707
   17  H    7.033460   7.078941   8.261052   8.507127   7.619427
   18  H    4.966473   4.795816   6.297666   6.853057   6.280684
   19  H    6.384597   7.061119   7.062756   6.564217   5.260166
   20  H    7.547828   7.939242   8.524360   8.348357   7.177950
   21  H    2.138124   2.479232   1.086241   2.178993   3.416993
   22  H    3.388351   4.299846   2.171719   1.086599   2.128792
   23  H    3.891816   4.978876   3.416286   2.130378   1.080546
   24  C    5.029495   5.976687   5.247486   4.380742   3.004420
   25  H    5.949103   6.832597   6.283335   5.470597   4.095751
   26  O    5.360943   6.397262   5.261206   4.135340   2.830584
                 16         17         18         19         20
   16  H    0.000000
   17  H    4.716229   0.000000
   18  H    2.398725   2.477345   0.000000
   19  H    5.564008   4.278126   4.970760   0.000000
   20  H    5.880219   2.499137   4.297529   2.407055   0.000000
   21  H    4.717129   9.169587   7.079811   8.146634   9.562183
   22  H    5.881080   9.562249   7.939565   7.381907   9.290476
   23  H    5.554409   8.118376   7.040576   5.205738   7.347789
   24  C    5.399131   6.252587   5.945406   2.629666   4.944364
   25  H    5.937274   5.916927   6.057160   1.837426   4.243787
   26  O    6.232827   7.473994   7.051098   3.755771   6.123881
                 21         22         23         24         25
   21  H    0.000000
   22  H    2.499325   0.000000
   23  H    4.301685   2.441552   0.000000
   24  C    6.307241   5.014151   2.666354   0.000000
   25  H    7.354669   6.110789   3.742523   1.097915   0.000000
   26  O    6.246319   4.520505   2.082267   1.224778   1.984775
                 26
   26  O    0.000000
Stoichiometry    C15H10O
Framework group  C1[X(C15H10O)]
Deg. of freedom    72
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
---------------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.779869	-0.991467	0.000268
2	6	0	-2.612071	-1.705937	0.000505
3	6	0	-1.344381	-1.045392	0.000157
4	6	0	-1.272009	0.396554	-0.000457
5	6	0	-2.524569	1.096280	-0.000679
6	6	0	-3.725618	0.428760	-0.000332
7	6	0	-0.164335	-1.793589	0.000417
8	6	0	0.010973	1.032958	-0.000799
9	6	0	1.204693	0.246968	-0.000518
10	6	0	1.098036	-1.192118	0.000100
11	6	0	2.275344	-2.001469	0.000387
12	1	0	2.159404	-3.082387	0.000854
13	6	0	3.520633	-1.429432	0.000081
14	6	0	3.636250	-0.013002	-0.000534
15	6	0	2.524598	0.798935	-0.000825
16	1	0	-0.230501	-2.879373	0.000885
17	1	0	-4.740128	-1.498764	0.000535
18	1	0	-2.627666	-2.792883	0.000964
19	1	0	-2.551766	2.177297	-0.001127
20	1	0	-4.650570	0.998767	-0.000518
21	1	0	4.412942	-2.048870	0.000301
22	1	0	4.623184	0.441597	-0.000784
23	1	0	2.645056	1.872746	-0.001303
24	6	0	0.056497	2.512125	-0.001445
25	1	0	-0.917938	3.017970	0.002205
26	8	0	1.056618	3.219107	0.002505

```
 Rotational constants (GHZ):      0.9716636      0.4412146
0.3034319
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   324 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   324 basis functions,   552 primitive gaussians,   324 cartesian
basis functions
    54 alpha electrons       54 beta electrons
       nuclear repulsion energy       964.0901904045 Hartrees.
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   324 RedAO= T  NBF=   324
 NBsUse=   317 1.00D-06 NBFU=   317
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=        4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -652.867988952     A.U. after   19 cycles
            Convg  =    0.7665D-08             -V/T =  2.0097
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.000105277   -0.000679921    0.000000376
    2          6          -0.001183489   -0.000512663   -0.000000865
    3          6           0.001437696   -0.001432090    0.000030100
    4          6          -0.000629317    0.001780987   -0.000034725
    5          6          -0.000590038   -0.000704229   -0.000006794
    6          6           0.000136666    0.000340785   -0.000000466
    7          6          -0.000634040    0.001488460   -0.000010589
    8          6          -0.001578102    0.000672800   -0.000255876
    9          6          -0.000669472    0.000469395   -0.000017143
   10          6           0.000560680   -0.002365771    0.000023667
   11          6           0.000949478    0.000822011    0.000002384
```

```
   12          1           0.000068425   -0.000390617    0.000002135
   13          6          -0.000023295   -0.000142319    0.000001202
   14          6          -0.000530523   -0.000499933   -0.000002053
   15          6           0.001666125    0.001860396   -0.000019646
   16          1           0.000307387   -0.000475030   -0.000000599
   17          1          -0.000207470   -0.000267591    0.000000310
   18          1           0.000448401   -0.000158466    0.000003344
   19          1          -0.000315651    0.000100102   -0.000011448
   20          1          -0.000353229    0.000038460   -0.000000858
   21          1           0.000378993    0.000069168    0.000001680
   22          1           0.000253770    0.000290158    0.000000007
   23          1          -0.000288139   -0.000706087    0.000006559
   24          6           0.003048224   -0.000953806    0.000916867
   25          1          -0.002271361   -0.000556260   -0.000301350
   26          8          -0.000086994    0.001912063   -0.000326218
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.003048224 RMS     0.000829594


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.002315947 RMS     0.000504708
 Search for a local minimum.
 Step number   8 out of a maximum of 152
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  2  3  4  6  5
                                                       8  7
 Trust test=-2.47D-01 RLast= 4.72D-02 DXMaxT set to 1.50D-01
 Energy Rises -- skip Quadratic search.
 Quartic linear search produced a step of -0.55386.
 Iteration  1 RMS(Cart)=  0.00286776 RMS(Int)=  0.00000896
 Iteration  2 RMS(Cart)=  0.00001095 RMS(Int)=  0.00000190
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000190
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.58707   0.00016  -0.00005   0.00000  -0.00005
2.58702
    R2        2.68580   0.00061   0.00126   0.00000   0.00126
2.68706
    R3        2.05229   0.00033   0.00070   0.00000   0.00070
2.05299
    R4        2.70129   0.00123   0.00249   0.00000   0.00249
2.70378
    R5        2.05424   0.00037   0.00107   0.00000   0.00107
2.05531
    R6        2.72831   0.00208   0.00582   0.00000   0.00582
2.73414
    R7        2.64042   0.00038  -0.00011   0.00000  -0.00011
2.64031
```

This journal is © The Royal Society of Chemistry 2014

R8	2.71129	0.00115	0.00183	0.00000	0.00182
2.71312					
R9	2.70637	0.00127	0.00166	0.00000	0.00166
2.70803					
R10	2.59664	0.00036	0.00038	0.00000	0.00038
2.59702					
R11	2.04347	0.00027	0.00100	0.00000	0.00100
2.04447					
R12	2.05315	0.00035	0.00095	0.00000	0.00095
2.05411					
R13	2.64247	-0.00011	-0.00101	0.00000	-0.00101
2.64147					
R14	2.05564	0.00057	0.00182	0.00000	0.00182
2.05746					
R15	2.70089	0.00140	0.00283	0.00000	0.00283
2.70372					
R16	2.79654	-0.00020	-0.00230	0.00000	-0.00230
2.79424					
R17	2.72694	0.00161	0.00372	0.00000	0.00372
2.73066					
R18	2.70357	0.00123	0.00371	0.00000	0.00371
2.70729					
R19	2.69980	0.00112	0.00230	0.00000	0.00230
2.70210					
R20	2.05436	0.00038	0.00108	0.00000	0.00108
2.05543					
R21	2.58966	0.00016	-0.00025	0.00000	-0.00025
2.58941					
R22	2.68557	0.00029	0.00109	0.00000	0.00109
2.68666					
R23	2.05270	0.00038	0.00093	0.00000	0.00093
2.05362					
R24	2.60139	-0.00001	-0.00114	0.00000	-0.00114
2.60024					
R25	2.05337	0.00038	0.00107	0.00000	0.00107
2.05445					
R26	2.04194	-0.00034	-0.00008	0.00000	-0.00009
2.04185					
R27	3.93492	0.00029	-0.01094	0.00000	-0.01094
3.92397					
R28	2.07476	0.00232	0.00654	0.00000	0.00654
2.08130					
R29	2.31450	0.00183	0.00129	0.00000	0.00129
2.31579					
A1	2.08167	-0.00025	-0.00169	0.00000	-0.00169
2.07998					
A2	2.10651	0.00019	0.00152	0.00000	0.00151
2.10803					
A3	2.09500	0.00007	0.00018	0.00000	0.00018
2.09518					
A4	2.11218	0.00032	0.00139	0.00000	0.00139
2.11357					

This journal is © The Royal Society of Chemistry 2014

A5	2.10551	0.00014	0.00220	0.00000	0.00220
2.10771					
A6	2.06550	-0.00046	-0.00359	0.00000	-0.00359
2.06190					
A7	2.10130	-0.00004	0.00013	0.00000	0.00013
2.10143					
A8	2.09616	0.00009	0.00020	0.00000	0.00020
2.09637					
A9	2.08572	-0.00005	-0.00033	0.00000	-0.00033
2.08539					
A10	2.03010	-0.00079	-0.00285	0.00000	-0.00285
2.02724					
A11	2.08142	-0.00033	-0.00147	0.00000	-0.00146
2.07995					
A12	2.17167	0.00112	0.00432	0.00000	0.00432
2.17599					
A13	2.12487	0.00035	0.00138	0.00000	0.00138
2.12625					
A14	2.10540	0.00003	0.00021	0.00000	0.00021
2.10561					
A15	2.05291	-0.00038	-0.00159	0.00000	-0.00159
2.05133					
A16	2.11625	0.00041	0.00164	0.00000	0.00164
2.11789					
A17	2.08490	-0.00015	-0.00020	0.00000	-0.00020
2.08470					
A18	2.08204	-0.00026	-0.00144	0.00000	-0.00144
2.08059					
A19	2.13188	0.00074	0.00304	0.00000	0.00304
2.13492					
A20	2.07501	-0.00034	-0.00177	0.00000	-0.00177
2.07323					
A21	2.07630	-0.00040	-0.00127	0.00000	-0.00127
2.07503					
A22	2.09884	-0.00025	-0.00026	0.00000	-0.00026
2.09858					
A23	2.06203	0.00068	0.00085	0.00000	0.00085
2.06288					
A24	2.12231	-0.00043	-0.00060	0.00000	-0.00059
2.12172					
A25	2.07910	0.00030	0.00153	0.00000	0.00153
2.08063					
A26	2.16322	-0.00001	-0.00190	0.00000	-0.00190
2.16133					
A27	2.04086	-0.00029	0.00037	0.00000	0.00037
2.04123					
A28	2.08942	-0.00041	-0.00252	0.00000	-0.00252
2.08690					
A29	2.09469	0.00076	0.00423	0.00000	0.00423
2.09892					
A30	2.09908	-0.00035	-0.00171	0.00000	-0.00171
2.09737					

This journal is © The Royal Society of Chemistry 2014

```
   A31        2.06620  -0.00022  -0.00147   0.00000  -0.00147
2.06474
   A32        2.10872   0.00018   0.00048   0.00000   0.00048
2.10921
   A33        2.10826   0.00003   0.00098   0.00000   0.00098
2.10924
   A34        2.08285   0.00008   0.00090   0.00000   0.00090
2.08375
   A35        2.10416   0.00003   0.00036   0.00000   0.00036
2.10452
   A36        2.09617  -0.00012  -0.00126   0.00000  -0.00126
2.09491
   A37        2.12018   0.00029   0.00047   0.00000   0.00047
2.12065
   A38        2.08389  -0.00022  -0.00156   0.00000  -0.00156
2.08233
   A39        2.07911  -0.00008   0.00109   0.00000   0.00109
2.08021
   A40        2.11468   0.00008  -0.00051   0.00000  -0.00051
2.11416
   A41        2.07859  -0.00087  -0.00828   0.00000  -0.00828
2.07032
   A42        2.08992   0.00079   0.00879   0.00000   0.00879
2.09871
   A43        2.01885  -0.00080  -0.00438   0.00000  -0.00437
2.01447
   A44        2.21690   0.00097   0.00473   0.00000   0.00475
2.22164
   A45        2.04741  -0.00017  -0.00036   0.00000  -0.00035
2.04707
    D1        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D2        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
    D3       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
    D4        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D5        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D6       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
    D7        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
    D8        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D9        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D10        3.14159   0.00001   0.00001   0.00000   0.00001  -
3.14159
   D11        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
```

This journal is © The Royal Society of Chemistry 2014

D12	-0.00001	0.00000	0.00001	0.00000	0.00001
0.00000					
D13	0.00001	0.00000	-0.00001	0.00000	-0.00001
0.00000					
D14	-3.14159	0.00000	-0.00001	0.00000	-0.00001
3.14159					
D15	-3.14158	-0.00001	-0.00001	0.00000	-0.00001
3.14159					
D16	0.00001	-0.00001	-0.00001	0.00000	-0.00001
-					
0.00001					
D17	-3.14159	-0.00001	-0.00001	0.00000	-0.00001
3.14159					
D18	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D19	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D20	3.14159	0.00000	0.00001	0.00000	0.00001
-					
3.14159					
D21	-0.00001	0.00000	0.00001	0.00000	0.00001
0.00000					
D22	3.14158	0.00001	0.00001	0.00000	0.00001
-					
3.14159					
D23	3.14159	0.00000	0.00001	0.00000	0.00001
-					
3.14159					
D24	-0.00001	0.00001	0.00001	0.00000	0.00001
0.00000					
D25	-0.00001	0.00002	0.00003	0.00000	0.00003
0.00001					
D26	3.14158	0.00002	0.00003	0.00000	0.00003
-					
3.14158					
D27	3.14158	0.00002	0.00003	0.00000	0.00003
-					
3.14158					
D28	-0.00002	0.00002	0.00003	0.00000	0.00003
0.00001					
D29	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D30	-3.14159	0.00000	0.00000	0.00000	0.00000
-					
3.14159					
D31	-3.14159	0.00000	-0.00001	0.00000	-0.00001
3.14159					
D32	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D33	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D34	3.14159	0.00000	0.00001	0.00000	0.00001
-					
3.14159					
D35	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D36	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D37	0.00001	-0.00002	-0.00002	0.00000	-0.00002
-					
0.00001					

This journal is © The Royal Society of Chemistry 2014

D38	-3.14159	-0.00001	-0.00001	0.00000	-0.00001
3.14158					
D39	-3.14158	-0.00002	-0.00002	0.00000	-0.00002
3.14158					
D40	0.00000	-0.00001	-0.00001	0.00000	-0.00001
-0.00001					
D41	0.00386	-0.00028	-0.00481	0.00000	-0.00481
-0.00095					
D42	3.13719	0.00030	0.00527	0.00000	0.00527
-3.14073					
D43	-3.13773	-0.00028	-0.00481	0.00000	-0.00481
3.14065					
D44	-0.00441	0.00030	0.00527	0.00000	0.00527
0.00086					
D45	0.00000	0.00001	0.00001	0.00000	0.00001
0.00000					
D46	3.14159	0.00000	0.00001	0.00000	0.00001
-3.14159					
D47	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D48	0.00001	0.00000	0.00000	0.00000	0.00000
0.00000					
D49	-3.14159	0.00000	-0.00001	0.00000	-0.00001
3.14159					
D50	-0.00001	0.00000	0.00000	0.00000	0.00000
0.00000					
D51	-0.00001	0.00000	0.00000	0.00000	0.00000
0.00000					
D52	3.14158	0.00000	0.00001	0.00000	0.00001
3.14159					
D53	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D54	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D55	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D56	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D57	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D58	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D59	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D60	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D61	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D62	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D63	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					

```
   D64        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D65        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D66       -3.14158   0.00000  -0.00001   0.00000  -0.00001  -
3.14159
   D67        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D68        0.00001   0.00000  -0.00001   0.00000  -0.00001
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.002316     0.000450     NO
 RMS     Force            0.000505     0.000300     NO
 Maximum Displacement     0.011393     0.001800     NO
 RMS     Displacement     0.002866     0.001200     NO
 Predicted change in Energy=-3.499563D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -6.634018   -4.462751    0.011127
    2          6             0       -5.266075   -4.409319    0.016000
    3          6             0       -4.575430   -3.156269    0.014877
    4          6             0       -5.314853   -1.912659    0.008526
    5          6             0       -6.745976   -2.027370    0.003600
    6          6             0       -7.375076   -3.249209    0.004857
    7          6             0       -3.178580   -3.125766    0.019920
    8          6             0       -4.596334   -0.672781    0.007549
    9          6             0       -3.165600   -0.669099    0.012786
   10          6             0       -2.457169   -1.928509    0.019069
   11          6             0       -1.027433   -1.948763    0.024376
   12          1             0       -0.525390   -2.913646    0.029041
   13          6             0       -0.308203   -0.782437    0.023604
   14          6             0       -0.996355    0.461626    0.017437
   15          6             0       -2.370966    0.522957    0.012213
   16          1             0       -2.633579   -4.068291    0.024676
   17          1             0       -7.153144   -5.417090    0.012007
   18          1             0       -4.673730   -5.321475    0.020843
   19          1             0       -7.369985   -1.143587   -0.001277
   20          1             0       -8.461415   -3.286508    0.000972
   21          1             0        0.778327   -0.802919    0.027652
   22          1             0       -0.424399    1.386178    0.016829
   23          1             0       -2.873086    1.479689    0.007568
   24          6             0       -5.373595    0.585084    0.001035
   25          1             0       -6.468324    0.464368   -0.003571
   26          8             0       -4.934500    1.729175   -0.001527
 ---------------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.368994	0.000000			
3	C	2.438174	1.430778	0.000000		
4	C	2.871092	2.497148	1.446843	0.000000	
5	C	2.437964	2.804271	2.446591	1.435721	0.000000
6	C	1.421932	2.407044	2.801206	2.455788	1.374284
7	C	3.705085	2.450543	1.397192	2.456709	3.732700
8	C	4.303026	3.796095	2.483586	1.433027	2.540843
9	C	5.140206	4.289668	2.858958	2.483092	3.829370
10	C	4.885541	3.747583	2.448355	2.857747	4.289974
11	C	6.144437	4.901071	3.747859	4.287602	5.719121
12	H	6.302014	4.971046	4.057325	4.892990	6.283455
13	C	7.318524	6.142868	4.883070	5.132657	6.557070
14	C	7.485504	6.477393	5.089101	4.928157	6.265256
15	C	6.559793	5.719179	4.289099	3.820825	5.064084
16	H	4.019862	2.654508	2.145382	3.440384	4.591036
17	H	1.086396	2.139310	3.428692	3.957318	3.414097
18	H	2.140147	1.087624	2.167445	3.468605	3.891738
19	H	3.399801	3.884809	3.443935	2.194341	1.081889
20	H	2.173254	3.386905	3.888192	3.433420	2.127950
21	H	8.266650	7.038541	5.848174	6.193443	7.623319
22	H	8.530496	7.551795	6.153445	5.899062	7.184345
23	H	7.032581	6.356640	4.938636	4.179742	5.224820
24	C	5.202826	4.995582	3.825569	2.498445	2.950992
25	H	4.929925	5.019821	4.085633	2.642138	2.507169
26	O	6.420939	6.147467	4.898649	3.661656	4.170504

		6	7	8	9	10
6	C	0.000000				
7	C	4.198338	0.000000			
8	C	3.789379	2.833251	0.000000		
9	C	4.937278	2.456712	1.430748	0.000000	
10	C	5.092176	1.397805	2.480527	1.445001	0.000000
11	C	6.479515	2.452099	3.790180	2.491874	1.429890
12	H	6.857942	2.661671	4.646990	3.465395	2.168493
13	C	7.485052	3.705437	4.289563	2.859664	2.435479
14	C	7.379602	4.198987	3.774497	2.446259	2.801201
15	C	6.266610	3.737041	2.526276	1.432634	2.452991
16	H	4.811765	1.088762	3.922013	3.440596	2.147049
17	H	2.179224	4.587743	5.389412	6.200317	5.849994
18	H	3.404675	2.656429	4.649357	4.890719	4.052822
19	H	2.105637	4.636524	2.813339	4.231098	4.975166
20	H	1.086987	5.285314	4.665883	5.907337	6.155929
21	H	8.512510	4.588332	5.376274	3.946225	3.425706
22	H	8.354571	5.286129	4.652359	3.426129	3.888356
23	H	6.529195	4.615592	2.757301	2.168612	3.433501
24	C	4.325245	4.311479	1.478649	2.539361	3.850197
25	H	3.822685	4.869499	2.190337	3.491847	4.670731
26	O	5.544435	5.162767	2.425661	2.980088	4.417719

		11	12	13	14	15
11	C	0.000000				

```
   12  H    1.087689   0.000000
   13  C    1.370258   2.142254   0.000000
   14  C    2.410599   3.407990   1.421718   0.000000
   15  C    2.813295   3.900855   2.441142   1.375989   0.000000
   16  H    2.659343   2.403681   4.025446   4.816711   4.598769
   17  H    7.039445   7.084817   8.266399   8.512660   7.625836
   18  H    4.966960   4.796503   6.297675   6.853274   6.281734
   19  H    6.393507   7.069830   7.071054   6.572687   5.269510
   20  H    7.553424   7.944829   8.529112   8.353198   7.183712
   21  H    2.138630   2.480897   1.086731   2.179145   3.417051
   22  H    3.389032   4.301027   2.171736   1.087166   2.129389
   23  H    3.893712   4.981317   3.419955   2.135105   1.080501
   24  C    5.030909   5.978878   5.246791   4.379012   3.003292
   25  H    5.952081   6.835970   6.285089   5.472010   4.097806
   26  O    5.365917   6.402887   5.264166   4.137152   2.833170
                 16         17         18         19         20
   16  H    0.000000
   17  H    4.716554   0.000000
   18  H    2.394307   2.481272   0.000000
   19  H    5.566696   4.279022   4.972427   0.000000
   20  H    5.880087   2.500215   4.299772   2.404857   0.000000
   21  H    4.722687   9.176004   7.081125   8.155481   9.567747
   22  H    5.884877   9.568724   7.940368   7.391968   9.296660
   23  H    5.553174   8.116925   7.035505   5.206126   7.344801
   24  C    5.400199   6.260432   5.947911   2.640811   4.952158
   25  H    5.937260   5.921213   6.057816   1.843506   4.247529
   26  O    6.237430   7.482758   7.055506   3.766211   6.131576
                 21         22         23         24         25
   21  H    0.000000
   22  H    2.497761   0.000000
   23  H    4.306219   2.450490   0.000000
   24  C    6.306616   5.013635   2.655730   0.000000
   25  H    7.356693   6.113851   3.735871   1.101374   0.000000
   26  O    6.248899   4.523162   2.076476   1.225461   1.988054
                 26
   26  O    0.000000
Stoichiometry    C15H10O
Framework group  C1[X(C15H10O)]
Deg. of freedom    72
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0        3.783542   -0.992231    0.000054
   2          6             0        2.614963   -1.705372    0.000096
   3          6             0        1.345929   -1.044555    0.000027
   4          6             0        1.272838    0.400440   -0.000090
   5          6             0        2.527961    1.097550   -0.000129
```

```
     6          6           0        3.728464    0.428633   -0.000059
     7          6           0        0.165981   -1.792796    0.000074
     8          6           0       -0.012109    1.034852   -0.000161
     9          6           0       -1.205417    0.245512   -0.000102
    10          6           0       -1.097769   -1.195474    0.000016
    11          6           0       -2.276990   -2.004191    0.000073
    12          1           0       -2.160617   -3.085637    0.000160
    13          6           0       -3.521792   -1.431414    0.000020
    14          6           0       -3.637825   -0.014439   -0.000092
    15          6           0       -2.527253    0.797950   -0.000151
    16          1           0        0.234202   -2.879419    0.000164
    17          1           0        4.744328   -1.499329    0.000107
    18          1           0        2.626946   -2.792930    0.000183
    19          1           0        2.558057    2.179020   -0.000214
    20          1           0        4.653638    0.999241   -0.000092
    21          1           0       -4.415124   -2.050238    0.000064
    22          1           0       -4.626101    0.438597   -0.000133
    23          1           0       -2.639046    1.872652   -0.000235
    24          6           0       -0.061591    2.512673   -0.000298
    25          1           0        0.916768    3.018476    0.000608
    26          8           0       -1.060831    3.222091    0.000465
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9703572      0.4405129
0.3029725
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   324 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   324 basis functions,   552 primitive gaussians,   324 cartesian
basis functions
    54 alpha electrons       54 beta electrons
       nuclear repulsion energy       963.4674048503 Hartrees.
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   324 RedAO= T  NBF=   324
 NBsUse=   317 1.00D-06 NBFU=   317
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB+HF-LYP) = -652.868042690 A.U. after 16 cycles
Convg = 0.7991D-08 -V/T = 2.0097
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000012547	-0.000083202	0.000000770
2	6	-0.000094012	-0.000065997	-0.000000614
3	6	-0.000055376	-0.000022231	-0.000004615
4	6	0.000072293	-0.000057683	0.000005742
5	6	-0.000095285	-0.000035967	0.000001410
6	6	0.000023125	0.000047883	-0.000000140
7	6	0.000032659	0.000061633	0.000000592
8	6	-0.000199671	-0.000037563	0.000053470
9	6	-0.000017931	0.000197829	0.000002940
10	6	0.000110202	-0.000116991	-0.000002394
11	6	0.000062963	0.000043535	-0.000000241
12	1	0.000006704	-0.000011504	-0.000000129
13	6	0.000034579	0.000105995	-0.000000188
14	6	0.000080718	-0.000117633	0.000000909
15	6	-0.000199974	0.000077510	0.000002865
16	1	0.000035437	-0.000007191	0.000001010
17	1	-0.000007270	-0.000034536	0.000000027
18	1	0.000015628	-0.000008990	-0.000000138
19	1	-0.000028378	0.000009134	0.000002266
20	1	-0.000014191	0.000003724	-0.000000261
21	1	0.000026574	0.000001307	0.000000031
22	1	-0.000026258	0.000034808	-0.000000313
23	1	0.000536481	-0.000171226	0.000001760
24	6	0.000170215	-0.000294314	-0.000197891

```
   25          1          -0.000317601   -0.000140645    0.000064781
   26          8          -0.000139085    0.000622315    0.000068353
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000622315 RMS     0.000127068


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000621710 RMS     0.000084286
 Search for a local minimum.
 Step number   9 out of a maximum of 152
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  2  3  4  6  5
                                                      8  7  9
     Eigenvalues ---    0.00237   0.01524   0.02056   0.02070
0.02082
     Eigenvalues ---    0.02085   0.02086   0.02088   0.02092
0.02096
     Eigenvalues ---    0.02229   0.02231   0.02253   0.02258
0.02348
     Eigenvalues ---    0.02349   0.02374   0.02381   0.02396
0.02424
     Eigenvalues ---    0.02429   0.02501   0.02504   0.07121
0.14887
     Eigenvalues ---    0.15980   0.15992   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16002   0.16017   0.16348   0.16680
0.21521
     Eigenvalues ---    0.21987   0.22185   0.22566   0.22885
0.23229
     Eigenvalues ---    0.24326   0.24679   0.24925   0.25656
0.30646
     Eigenvalues ---    0.35858   0.36886   0.37221   0.37230
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37271   0.37354
0.37419
     Eigenvalues ---    0.37675   0.40754   0.42219   0.43001
0.43567
     Eigenvalues ---    0.43641   0.44755   0.45323   0.45395
0.45720
     Eigenvalues ---    0.46654   0.51569   0.51572   0.52738
0.55728
     Eigenvalues ---    0.57695
0.803791000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-8.42992497D-06.
 Quartic linear search produced a step of -0.00261.
 Iteration  1 RMS(Cart)=  0.00130061 RMS(Int)=  0.00000136
 Iteration  2 RMS(Cart)=  0.00000155 RMS(Int)=  0.00000012
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000012
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.58702   0.00002   0.00000  -0.00003  -0.00003
2.58700
    R2        2.68706   0.00006   0.00000   0.00010   0.00010
2.68716
    R3        2.05299   0.00003   0.00000   0.00006   0.00006
2.05305
    R4        2.70378   0.00015   0.00001   0.00028   0.00029
2.70407
    R5        2.05531   0.00001   0.00000   0.00003   0.00003
2.05534
    R6        2.73414   0.00006   0.00001   0.00020   0.00021
2.73435
    R7        2.64031   0.00017   0.00000   0.00016   0.00016
2.64047
    R8        2.71312   0.00012   0.00000   0.00027   0.00028
2.71340
    R9        2.70803   0.00016   0.00000   0.00042   0.00043
2.70846
   R10        2.59702   0.00001   0.00000   0.00000   0.00000
2.59703
   R11        2.04447   0.00003   0.00000   0.00005   0.00005
2.04452
```

This journal is © The Royal Society of Chemistry 2014

R12	2.05411	0.00002	0.00000	0.00003	0.00003
2.05414					
R13	2.64147	0.00006	0.00000	0.00007	0.00007
2.64153					
R14	2.05746	0.00002	0.00000	0.00007	0.00007
2.05753					
R15	2.70372	0.00016	0.00001	0.00046	0.00047
2.70419					
R16	2.79424	0.00008	0.00000	0.00041	0.00040
2.79464					
R17	2.73066	0.00015	0.00001	0.00057	0.00058
2.73124					
R18	2.70729	-0.00001	0.00001	0.00013	0.00014
2.70743					
R19	2.70210	0.00012	0.00000	0.00025	0.00026
2.70236					
R20	2.05543	0.00002	0.00000	0.00003	0.00003
2.05547					
R21	2.58941	0.00003	0.00000	-0.00010	-0.00010
2.58931					
R22	2.68666	-0.00008	0.00000	-0.00030	-0.00030
2.68636					
R23	2.05362	0.00003	0.00000	0.00004	0.00004
2.05366					
R24	2.60024	0.00007	0.00000	0.00014	0.00014
2.60038					
R25	2.05445	0.00001	0.00000	0.00002	0.00002
2.05447					
R26	2.04185	-0.00020	0.00000	-0.00093	-0.00093
2.04092					
R27	3.92397	0.00036	-0.00002	0.01571	0.01569
3.93966					
R28	2.08130	0.00033	0.00001	0.00081	0.00083
2.08212					
R29	2.31579	0.00062	0.00000	0.00052	0.00052
2.31631					
A1	2.07998	-0.00004	0.00000	-0.00034	-0.00034
2.07964					
A2	2.10803	0.00001	0.00000	0.00018	0.00018
2.10821					
A3	2.09518	0.00003	0.00000	0.00016	0.00016
2.09533					
A4	2.11357	0.00003	0.00000	0.00013	0.00013
2.11371					
A5	2.10771	-0.00001	0.00000	0.00014	0.00014
2.10785					
A6	2.06190	-0.00002	-0.00001	-0.00027	-0.00028
2.06163					
A7	2.10143	-0.00001	0.00000	0.00021	0.00021
2.10163					
A8	2.09637	0.00004	0.00000	0.00009	0.00009
2.09645					

A9	2.08539	-0.00003	0.00000	-0.00030	-0.00030
2.08510					
A10	2.02724	-0.00004	-0.00001	-0.00042	-0.00043
2.02682					
A11	2.07995	0.00002	0.00000	0.00018	0.00018
2.08013					
A12	2.17599	0.00002	0.00001	0.00024	0.00025
2.17624					
A13	2.12625	0.00002	0.00000	0.00014	0.00015
2.12640					
A14	2.10561	0.00001	0.00000	0.00025	0.00025
2.10586					
A15	2.05133	-0.00003	0.00000	-0.00040	-0.00040
2.05093					
A16	2.11789	0.00004	0.00000	0.00027	0.00028
2.11817					
A17	2.08470	-0.00001	0.00000	0.00000	0.00000
2.08471					
A18	2.08059	-0.00003	0.00000	-0.00028	-0.00028
2.08031					
A19	2.13492	0.00007	0.00001	0.00037	0.00038
2.13530					
A20	2.07323	-0.00001	0.00000	0.00002	0.00001
2.07325					
A21	2.07503	-0.00006	0.00000	-0.00039	-0.00039
2.07464					
A22	2.09858	-0.00002	0.00000	0.00000	0.00000
2.09858					
A23	2.06288	0.00011	0.00000	-0.00058	-0.00058
2.06230					
A24	2.12172	-0.00009	0.00000	0.00058	0.00058
2.12230					
A25	2.08063	0.00002	0.00000	-0.00022	-0.00021
2.08041					
A26	2.16133	0.00008	0.00000	0.00127	0.00126
2.16259					
A27	2.04123	-0.00010	0.00000	-0.00105	-0.00105
2.04018					
A28	2.08690	-0.00005	-0.00001	-0.00004	-0.00005
2.08685					
A29	2.09892	0.00004	0.00001	-0.00047	-0.00046
2.09846					
A30	2.09737	0.00001	0.00000	0.00052	0.00051
2.09788					
A31	2.06474	-0.00002	0.00000	-0.00031	-0.00031
2.06443					
A32	2.10921	0.00003	0.00000	0.00022	0.00022
2.10943					
A33	2.10924	-0.00001	0.00000	0.00009	0.00009
2.10933					
A34	2.08375	-0.00006	0.00000	-0.00061	-0.00061
2.08314					

This journal is © The Royal Society of Chemistry 2014

A35	2.10452	0.00003	0.00000	0.00036	0.00036
2.10488					
A36	2.09491	0.00003	0.00000	0.00026	0.00025
2.09516					
A37	2.12065	0.00007	0.00000	0.00050	0.00050
2.12115					
A38	2.08233	0.00000	0.00000	0.00011	0.00011
2.08244					
A39	2.08021	-0.00007	0.00000	-0.00061	-0.00061
2.07960					
A40	2.11416	0.00005	0.00000	0.00043	0.00043
2.11459					
A41	2.07032	0.00007	-0.00002	0.00268	0.00266
2.07298					
A42	2.09871	-0.00013	0.00002	-0.00311	-0.00309
2.09561					
A43	2.01447	-0.00014	-0.00001	-0.00134	-0.00135
2.01313					
A44	2.22164	0.00007	0.00001	0.00101	0.00102
2.22267					
A45	2.04707	0.00007	0.00000	0.00033	0.00032
2.04739					
D1	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D2	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D3	3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D4	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D5	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D6	3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D7	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D8	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D9	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D10	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D11	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D12	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D13	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D14	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D15	3.14159	0.00000	0.00000	0.00001	0.00001	-
3.14159					

This journal is © The Royal Society of Chemistry 2014

D16	-0.00001	0.00000	0.00000	0.00000	0.00000
0.00000					
D17	3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D18	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D19	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D20	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D21	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D22	-3.14159	0.00000	0.00000	-0.00001	-0.00001
3.14159					
D23	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D24	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D25	0.00001	0.00000	0.00000	-0.00001	-0.00001
0.00000					
D26	-3.14158	0.00000	0.00000	-0.00002	-0.00002
3.14159					
D27	-3.14158	0.00000	0.00000	-0.00001	-0.00001
3.14159					
D28	0.00001	0.00000	0.00000	-0.00002	-0.00002
-0.00001					
D29	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D30	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D31	3.14159	0.00000	0.00000	0.00001	0.00001
-3.14159					
D32	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D33	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D34	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D35	3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D36	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D37	-0.00001	0.00000	0.00000	0.00001	0.00001
0.00000					
D38	3.14158	0.00000	0.00000	0.00001	0.00001
3.14159					
D39	3.14158	0.00000	0.00000	0.00002	0.00002
-3.14159					
D40	-0.00001	0.00000	0.00000	0.00002	0.00002
0.00000					
D41	-0.00095	0.00006	-0.00001	0.00084	0.00083
-0.00012					

D42	-3.14073	-0.00007	0.00001	-0.00083	-0.00082	-3.14155
D43	3.14065	0.00006	-0.00001	0.00083	0.00082	3.14147
D44	0.00086	-0.00007	0.00001	-0.00084	-0.00083	0.00004
D45	0.00000	0.00000	0.00000	-0.00001	-0.00001	0.00000
D46	-3.14159	0.00000	0.00000	-0.00001	-0.00001	3.14159
D47	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D48	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D49	3.14159	0.00000	0.00000	0.00001	0.00001	-3.14159
D50	0.00000	0.00000	0.00000	0.00001	0.00001	0.00001
D51	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D52	3.14159	0.00000	0.00000	0.00001	0.00001	-3.14159
D53	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D54	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D55	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D56	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D57	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D58	-3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D59	3.14159	0.00000	0.00000	0.00000	0.00000	3.14159
D60	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D61	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D62	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D63	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159
D64	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D65	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D66	-3.14159	0.00000	0.00000	-0.00001	-0.00001	3.14159
D67	-3.14159	0.00000	0.00000	0.00000	0.00000	-3.14159

```
   D68        0.00000   0.00000   0.00000  -0.00001  -0.00001  -
0.00001
         Item               Value     Threshold  Converged?
 Maximum Force            0.000622     0.000450     NO
 RMS     Force            0.000084     0.000300     YES
 Maximum Displacement     0.009243     0.001800     NO
 RMS     Displacement     0.001300     0.001200     NO
 Predicted change in Energy=-4.214147D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -6.634029   -4.463238    0.011133
    2          6             0       -5.266121   -4.409311    0.016037
    3          6             0       -4.575687   -3.155970    0.014867
    4          6             0       -5.315189   -1.912278    0.008430
    5          6             0       -6.746406   -2.027640    0.003477
    6          6             0       -7.375142   -3.249668    0.004782
    7          6             0       -3.178762   -3.125026    0.019949
    8          6             0       -4.596798   -0.672065    0.007405
    9          6             0       -3.165818   -0.668097    0.012694
   10          6             0       -2.457255   -1.927786    0.019062
   11          6             0       -1.027393   -1.948796    0.024418
   12          1             0       -0.526153   -2.914114    0.029143
   13          6             0       -0.307320   -0.783053    0.023617
   14          6             0       -0.995228    0.460964    0.017369
   15          6             0       -2.369873    0.523173    0.012096
   16          1             0       -2.633434   -4.067404    0.024771
   17          1             0       -7.152999   -5.417697    0.012049
   18          1             0       -4.673308   -5.321181    0.020944
   19          1             0       -7.371047   -1.144273   -0.001457
   20          1             0       -8.461499   -3.286990    0.000872
   21          1             0        0.779223   -0.803956    0.027702
   22          1             0       -0.423242    1.385512    0.016736
   23          1             0       -2.868195    1.481336    0.007407
   24          6             0       -5.375145    0.585379    0.000776
   25          1             0       -6.470053    0.462295   -0.003038
   26          8             0       -4.938011    1.730516   -0.001052
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                       1          2          3          4          5
    1  C    0.000000
    2  C    1.368980   0.000000
    3  C    2.438388   1.430930   0.000000
    4  C    2.871714   2.497526   1.446954   0.000000
    5  C    2.438201   2.804239   2.446483   1.435867   0.000000
    6  C    1.421985   2.406838   2.801041   2.456019   1.374287
```

This journal is © The Royal Society of Chemistry 2014

7	C	3.705369	2.450810	1.397277	2.456667	3.732641
8	C	4.303873	3.796719	2.484007	1.433254	2.541341
9	C	5.141166	4.290450	2.859589	2.483506	3.830020
10	C	4.886105	3.748025	2.448715	2.857996	4.290341
11	C	6.144670	4.901124	3.748033	4.287982	5.719595
12	H	6.301290	4.970219	4.056775	4.892747	6.283155
13	C	7.319233	6.143249	4.883623	5.133628	6.558295
14	C	7.486246	6.477662	5.089392	4.928938	6.266529
15	C	6.561046	5.719935	4.289723	3.821822	5.065645
16	H	4.020153	2.654809	2.145496	3.440443	4.591038
17	H	1.086426	2.139432	3.428987	3.957968	3.414363
18	H	2.140231	1.087639	2.167419	3.468831	3.891716
19	H	3.399835	3.884777	3.444014	2.194648	1.081914
20	H	2.173318	3.386780	3.888045	3.433533	2.127795
21	H	8.267220	7.038813	5.848692	6.194401	7.624505
22	H	8.531225	7.552049	6.153687	5.899715	7.185554
23	H	7.037008	6.360019	4.941679	4.183826	5.230052
24	C	5.203214	4.995903	3.825837	2.498389	2.950971
25	H	4.928282	5.018203	4.084212	2.640538	2.505232
26	O	6.421777	6.148611	4.899927	3.662281	4.170618

		6	7	8	9	10
6	C	0.000000				
7	C	4.198258	0.000000			
8	C	3.789886	2.833373	0.000000		
9	C	4.937913	2.456974	1.430996	0.000000	
10	C	5.092463	1.397839	2.480850	1.445309	0.000000
11	C	6.479705	2.451923	3.790908	2.492627	1.430027
12	H	6.857247	2.660997	4.647301	3.465933	2.168433
13	C	7.485897	3.705406	4.290944	2.860829	2.435705
14	C	7.380532	4.198470	3.775601	2.446684	2.800653
15	C	6.267942	3.736806	2.527412	1.432708	2.452527
16	H	4.811744	1.088799	3.922172	3.440766	2.146867
17	H	2.179392	4.588132	5.390288	6.201315	5.850601
18	H	3.404605	2.656458	4.649766	4.891195	4.052903
19	H	2.105408	4.636712	2.814164	4.232127	4.975908
20	H	1.087005	5.285253	4.666239	5.907874	6.156192
21	H	8.513266	4.588362	5.377677	3.947408	3.426056
22	H	8.355475	5.285627	4.653202	3.426230	3.887823
23	H	6.534139	4.616837	2.761377	2.169947	3.433821
24	C	4.325227	4.311794	1.478862	2.540171	3.851028
25	H	3.820722	4.868469	2.189969	3.492278	4.670709
26	O	5.544536	5.164464	2.426704	2.982315	4.420150

		11	12	13	14	15
11	C	0.000000				
12	H	1.087705	0.000000			
13	C	1.370205	2.142275	0.000000		
14	C	2.409985	3.407539	1.421561	0.000000	
15	C	2.813012	3.900582	2.441410	1.376062	0.000000
16	H	2.658547	2.402235	4.024646	4.815589	4.598155
17	H	7.039636	7.084017	8.267005	8.513332	7.627072
18	H	4.966457	4.795095	6.297338	6.852845	6.281908
19	H	6.394519	7.070067	7.073001	6.574816	5.271841

This journal is © The Royal Society of Chemistry 2014

20	H	7.553625	7.944152	8.529997	8.354198	7.185080
21	H	2.138815	2.481285	1.086752	2.179176	3.417356
22	H	3.388609	4.300875	2.171672	1.087179	2.129090
23	H	3.892897	4.980524	3.418450	2.132901	1.080011
24	C	5.032450	5.979965	5.249378	4.381715	3.005937
25	H	5.952870	6.836016	6.287358	5.474863	4.100660
26	O	5.369443	6.406090	5.268959	4.142178	2.837813

		16	17	18	19	20
16	H	0.000000				
17	H	4.716981	0.000000			
18	H	2.394380	2.481584	0.000000		
19	H	5.566898	4.279004	4.972410	0.000000	
20	H	5.880132	2.500442	4.299852	2.404230	0.000000
21	H	4.721899	9.176436	7.080640	8.157424	9.568548
22	H	5.883818	9.569394	7.939951	7.394062	9.297640
23	H	5.553732	8.121343	7.037958	5.212445	7.349967
24	C	5.400551	6.260815	5.948146	2.641085	4.951850
25	H	5.936210	5.919539	6.056192	1.841970	4.245351
26	O	6.239200	7.483535	7.056698	3.766176	6.131096

		21	22	23	24	25
21	H	0.000000				
22	H	2.497962	0.000000			
23	H	4.304257	2.446849	0.000000		
24	C	6.309296	5.016155	2.662251	0.000000	
25	H	7.359099	6.116915	3.743252	1.101811	0.000000
26	O	6.253890	4.527967	2.084778	1.225736	1.988855

		26	
26	O	0.000000	

Stoichiometry C15H10O
Framework group C1[X(C15H10O)]
Deg. of freedom 72
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.783424	-0.993997	0.000004
2	6	0	2.614395	-1.706372	0.000008
3	6	0	1.345566	-1.044832	0.000003
4	6	0	1.272909	0.400297	-0.000005
5	6	0	2.528670	1.096557	-0.000012
6	6	0	3.728783	0.426937	-0.000006
7	6	0	0.165096	-1.792410	0.000005
8	6	0	-0.011936	1.035427	-0.000012
9	6	0	-1.205833	0.246530	-0.000010
10	6	0	-1.098553	-1.194792	0.000000
11	6	0	-2.277692	-2.003871	0.000005
12	1	0	-2.160720	-3.085269	0.000013
13	6	0	-3.522710	-1.431690	0.000002

```
   14          6             0       -3.638514   -0.014854   -0.000005
   15          6             0       -2.528168    0.797967   -0.000011
   16          1             0        0.232652   -2.879111    0.000011
   17          1             0        4.744000   -1.501556    0.000007
   18          1             0        2.625517   -2.793954    0.000014
   19          1             0        2.559833    2.178022   -0.000024
   20          1             0        4.654147    0.997271   -0.000011
   21          1             0       -4.415996   -2.050616    0.000006
   22          1             0       -4.626683    0.438444   -0.000006
   23          1             0       -2.643608    1.871790   -0.000023
   24          6             0       -0.059857    2.513512   -0.000013
   25          1             0        0.920106    3.017159    0.000110
   26          8             0       -1.057840    3.225171    0.000024
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9696461      0.4404288
0.3028634
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   324 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   324 basis functions,   552 primitive gaussians,   324 cartesian
basis functions
    54 alpha electrons       54 beta electrons
       nuclear repulsion energy       963.3251563010 Hartrees.
 NAtoms=   26 NActive=   26 NUniq=   26 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   324 RedAO= T  NBF=   324
 NBsUse=   317 1.00D-06 NBFU=   317
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -652.868047290     A.U. after   14 cycles
            Convg  =    0.5591D-08             -V/T =  2.0097
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.000001797   -0.000004004    0.000000043
    2          6           0.000009428   -0.000011362    0.000000018
    3          6          -0.000018080    0.000054117   -0.000000669
    4          6           0.000078427   -0.000087175    0.000001301
    5          6          -0.000049874   -0.000005665   -0.000000039
    6          6          -0.000002182    0.000016498   -0.000000062
    7          6           0.000011773    0.000003207    0.000000153
    8          6          -0.000106983    0.000041649    0.000004019
    9          6           0.000049213    0.000090763    0.000000069
   10          6           0.000014293   -0.000043303   -0.000000126
   11          6          -0.000025745   -0.000033497    0.000000001
   12          1           0.000007313   -0.000001229    0.000000059
   13          6           0.000006550    0.000073344   -0.000000323
   14          6           0.000070766   -0.000065474    0.000000590
   15          6          -0.000022951   -0.000040328    0.000000722
   16          1           0.000005398   -0.000002733    0.000000045
   17          1           0.000006700   -0.000010573    0.000000042
   18          1          -0.000000452   -0.000009273    0.000000008
   19          1           0.000001607   -0.000003127    0.000000240
   20          1          -0.000004734   -0.000007014    0.000000013
   21          1           0.000003499   -0.000008207    0.000000013
   22          1          -0.000015056    0.000019953   -0.000000120
   23          1          -0.000004689    0.000030799   -0.000000379
   24          6           0.000074091   -0.000030667   -0.000017156
   25          1          -0.000033417    0.000017501    0.000005519
   26          8          -0.000056690    0.000015803    0.000006019
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000106983 RMS     0.000031735


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
```

This journal is © The Royal Society of Chemistry 2014

```
 Berny optimization.
 Internal  Forces:  Max     0.000068378 RMS     0.000015168
 Search for a local minimum.
 Step number  10 out of a maximum of 152
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  2  3  4  6  5
                                                     8  7  9 10
 Trust test= 1.09D+00 RLast= 1.67D-02 DXMaxT set to 1.50D-01
     Eigenvalues ---    0.00237   0.01524   0.02056   0.02070
0.02082
     Eigenvalues ---    0.02085   0.02086   0.02088   0.02092
0.02096
     Eigenvalues ---    0.02229   0.02231   0.02237   0.02253
0.02258
     Eigenvalues ---    0.02348   0.02349   0.02374   0.02381
0.02424
     Eigenvalues ---    0.02429   0.02501   0.02504   0.07102
0.14865
     Eigenvalues ---    0.15967   0.15994   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16002   0.16038   0.16579   0.16677
0.21537
     Eigenvalues ---    0.21980   0.22211   0.22559   0.22889
0.23264
     Eigenvalues ---    0.24254   0.24681   0.24940   0.25857
0.30857
     Eigenvalues ---    0.35806   0.36903   0.37226   0.37230
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37260   0.37371
0.37494
     Eigenvalues ---    0.37960   0.40724   0.42204   0.42983
0.43578
     Eigenvalues ---    0.43678   0.44766   0.45327   0.45413
0.45672
     Eigenvalues ---    0.46581   0.51560   0.51574   0.52732
0.55614
     Eigenvalues ---    0.57324
0.817841000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-9.76203648D-08.
 Quartic linear search produced a step of  0.06455.
 Iteration  1 RMS(Cart)=  0.00013998 RMS(Int)=  0.00000001
 Iteration  2 RMS(Cart)=  0.00000001 RMS(Int)=  0.00000001
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.58700   0.00001   0.00000   0.00001   0.00000
2.58700
    R2        2.68716   0.00001   0.00001   0.00002   0.00003
2.68719
    R3        2.05305   0.00001   0.00000   0.00001   0.00001
2.05306
    R4        2.70407   0.00002   0.00002   0.00001   0.00003
2.70409
    R5        2.05534   0.00001   0.00000   0.00001   0.00001
2.05535
    R6        2.73435  -0.00003   0.00001  -0.00011  -0.00010
2.73425
    R7        2.64047   0.00000   0.00001  -0.00003  -0.00002
2.64045
    R8        2.71340   0.00005   0.00002   0.00008   0.00010
2.71350
    R9        2.70846   0.00004   0.00003   0.00006   0.00009
2.70854
   R10        2.59703  -0.00001   0.00000  -0.00002  -0.00001
2.59701
   R11        2.04452   0.00000   0.00000   0.00000   0.00000
2.04452
   R12        2.05414   0.00001   0.00000   0.00001   0.00001
2.05415
   R13        2.64153  -0.00001   0.00000  -0.00004  -0.00003
2.64150
   R14        2.05753   0.00001   0.00000   0.00001   0.00001
2.05754
   R15        2.70419   0.00007   0.00003   0.00015   0.00018
2.70437
   R16        2.79464  -0.00001   0.00003  -0.00008  -0.00005
2.79459
```

This journal is © The Royal Society of Chemistry 2014

R17	2.73124	0.00005	0.00004	0.00011	0.00014
2.73138					
R18	2.70743	-0.00003	0.00001	-0.00007	-0.00006
2.70736					
R19	2.70236	0.00000	0.00002	-0.00003	-0.00001
2.70235					
R20	2.05547	0.00001	0.00000	0.00001	0.00002
2.05548					
R21	2.58931	0.00004	-0.00001	0.00006	0.00006
2.58937					
R22	2.68636	-0.00003	-0.00002	-0.00006	-0.00008
2.68628					
R23	2.05366	0.00000	0.00000	0.00000	0.00001
2.05367					
R24	2.60038	0.00006	0.00001	0.00010	0.00011
2.60049					
R25	2.05447	0.00001	0.00000	0.00002	0.00002
2.05449					
R26	2.04092	0.00005	-0.00006	0.00015	0.00009
2.04102					
R27	3.93966	0.00004	0.00101	0.00032	0.00133
3.94099					
R28	2.08212	0.00003	0.00005	0.00003	0.00008
2.08220					
R29	2.31631	0.00000	0.00003	-0.00004	-0.00001
2.31630					
A1	2.07964	0.00000	-0.00002	0.00003	0.00001
2.07965					
A2	2.10821	-0.00001	0.00001	-0.00006	-0.00005
2.10816					
A3	2.09533	0.00001	0.00001	0.00003	0.00004
2.09537					
A4	2.11371	0.00000	0.00001	-0.00002	-0.00001
2.11370					
A5	2.10785	-0.00001	0.00001	-0.00005	-0.00004
2.10781					
A6	2.06163	0.00001	-0.00002	0.00007	0.00005
2.06168					
A7	2.10163	0.00000	0.00001	0.00000	0.00002
2.10165					
A8	2.09645	-0.00001	0.00001	-0.00004	-0.00003
2.09642					
A9	2.08510	0.00001	-0.00002	0.00003	0.00002
2.08511					
A10	2.02682	0.00000	-0.00003	0.00003	0.00000
2.02682					
A11	2.08013	0.00002	0.00001	0.00008	0.00009
2.08022					
A12	2.17624	-0.00002	0.00002	-0.00011	-0.00009
2.17615					
A13	2.12640	0.00000	0.00001	-0.00001	0.00000
2.12640					

This journal is © The Royal Society of Chemistry 2014

A14	2.10586	0.00000	0.00002	-0.00002	0.00000
2.10586					
A15	2.05093	0.00000	-0.00003	0.00003	0.00001
2.05093					
A16	2.11817	-0.00001	0.00002	-0.00004	-0.00002
2.11815					
A17	2.08471	0.00000	0.00000	0.00000	0.00000
2.08470					
A18	2.08031	0.00001	-0.00002	0.00004	0.00002
2.08033					
A19	2.13530	0.00000	0.00002	-0.00003	-0.00001
2.13529					
A20	2.07325	0.00000	0.00000	0.00001	0.00002
2.07326					
A21	2.07464	0.00000	-0.00003	0.00002	-0.00001
2.07463					
A22	2.09858	-0.00003	0.00000	-0.00008	-0.00008
2.09850					
A23	2.06230	0.00004	-0.00004	0.00009	0.00006
2.06236					
A24	2.12230	-0.00002	0.00004	-0.00001	0.00002
2.12232					
A25	2.08041	-0.00001	-0.00001	-0.00006	-0.00007
2.08034					
A26	2.16259	0.00002	0.00008	0.00008	0.00017
2.16276					
A27	2.04018	-0.00001	-0.00007	-0.00003	-0.00009
2.04009					
A28	2.08685	0.00001	0.00000	0.00006	0.00006
2.08690					
A29	2.09846	-0.00001	-0.00003	-0.00009	-0.00012
2.09834					
A30	2.09788	0.00001	0.00003	0.00003	0.00007
2.09795					
A31	2.06443	0.00000	-0.00002	0.00003	0.00001
2.06444					
A32	2.10943	0.00000	0.00001	-0.00002	0.00000
2.10942					
A33	2.10933	0.00000	0.00001	-0.00002	-0.00001
2.10932					
A34	2.08314	-0.00001	-0.00004	-0.00002	-0.00006
2.08308					
A35	2.10488	-0.00001	0.00002	-0.00007	-0.00005
2.10483					
A36	2.09516	0.00002	0.00002	0.00010	0.00011
2.09528					
A37	2.12115	0.00001	0.00003	0.00005	0.00008
2.12123					
A38	2.08244	0.00001	0.00001	0.00010	0.00011
2.08255					
A39	2.07960	-0.00003	-0.00004	-0.00015	-0.00019
2.07941					

This journal is © The Royal Society of Chemistry 2014

A40	2.11459	0.00000	0.00003	-0.00002	0.00001
2.11461					
A41	2.07298	-0.00002	0.00017	-0.00007	0.00010
2.07308					
A42	2.09561	0.00002	-0.00020	0.00009	-0.00011
2.09550					
A43	2.01313	0.00002	-0.00009	0.00014	0.00005
2.01318					
A44	2.22267	0.00002	0.00007	0.00008	0.00014
2.22281					
A45	2.04739	-0.00003	0.00002	-0.00021	-0.00019
2.04720					
D1	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D2	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D3	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D4	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D5	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D6	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D7	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D8	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D9	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D10	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D11	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D12	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D13	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D14	3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D15	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D16	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D17	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D18	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D19	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D20	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					

This journal is © The Royal Society of Chemistry 2014

D21	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D22	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D23	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D24	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D25	0.00000	0.00000	0.00000	-0.00001	-0.00001
0.00000					
D26	3.14159	0.00000	0.00000	0.00000	0.00000
3.14158					
D27	3.14159	0.00000	0.00000	0.00000	0.00000
3.14158					
D28	-0.00001	0.00000	0.00000	0.00000	0.00000
0.00001					
D29	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D30	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D31	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D32	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D33	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D34	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D35	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D36	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D37	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D38	3.14159	0.00000	0.00000	0.00001	0.00001
3.14159					
D39	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14158					
D40	0.00000	0.00000	0.00000	0.00000	0.00000
0.00001					
D41	-0.00012	0.00001	0.00005	0.00000	0.00006
0.00006					
D42	-3.14155	-0.00001	-0.00005	-0.00005	-0.00011
3.14153					
D43	3.14147	0.00001	0.00005	0.00001	0.00006
3.14153					
D44	0.00004	-0.00001	-0.00005	-0.00005	-0.00010
0.00007					
D45	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D46	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					

This journal is © The Royal Society of Chemistry 2014

```
   D47       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D48        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D49       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D50        0.00001   0.00000   0.00000   0.00000   0.00000
0.00001
   D51        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D52       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D53        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D54        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D55        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D56        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D57        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D58        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D59        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D60        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D61        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D62       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D63       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D64        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D65        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D66        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D67       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D68       -0.00001   0.00000   0.00000   0.00000   0.00000
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.000068     0.000450     YES
 RMS     Force            0.000015     0.000300     YES
 Maximum Displacement     0.000769     0.001800     YES
 RMS     Displacement     0.000140     0.001200     YES
 Predicted change in Energy=-6.891505D-08
 Optimization completed.
    -- Stationary point found.
```

This journal is © The Royal Society of Chemistry 2014

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.369	-DE/DX = 0.0
R2	R(1,6)	1.422	-DE/DX = 0.0
R3	R(1,17)	1.0864	-DE/DX = 0.0
R4	R(2,3)	1.4309	-DE/DX = 0.0
R5	R(2,18)	1.0876	-DE/DX = 0.0
R6	R(3,4)	1.447	-DE/DX = 0.0
R7	R(3,7)	1.3973	-DE/DX = 0.0
R8	R(4,5)	1.4359	-DE/DX = 0.0
R9	R(4,8)	1.4333	-DE/DX = 0.0
R10	R(5,6)	1.3743	-DE/DX = 0.0
R11	R(5,19)	1.0819	-DE/DX = 0.0
R12	R(6,20)	1.087	-DE/DX = 0.0
R13	R(7,10)	1.3978	-DE/DX = 0.0
R14	R(7,16)	1.0888	-DE/DX = 0.0
R15	R(8,9)	1.431	-DE/DX = 0.0001
R16	R(8,24)	1.4789	-DE/DX = 0.0
R17	R(9,10)	1.4453	-DE/DX = 0.0001
R18	R(9,15)	1.4327	-DE/DX = 0.0
R19	R(10,11)	1.43	-DE/DX = 0.0
R20	R(11,12)	1.0877	-DE/DX = 0.0
R21	R(11,13)	1.3702	-DE/DX = 0.0

This journal is © The Royal Society of Chemistry 2014

```
 ! R22   R(13,14)                1.4216         -DE/DX =    0.0
!
 ! R23   R(13,21)                1.0868         -DE/DX =    0.0
!
 ! R24   R(14,15)                1.3761         -DE/DX =    0.0001
!
 ! R25   R(14,22)                1.0872         -DE/DX =    0.0
!
 ! R26   R(15,23)                1.08           -DE/DX =    0.0
!
 ! R27   R(23,26)                2.0848         -DE/DX =    0.0
!
 ! R28   R(24,25)                1.1018         -DE/DX =    0.0
!
 ! R29   R(24,26)                1.2257         -DE/DX =    0.0
!
 ! A1    A(2,1,6)               119.1548        -DE/DX =    0.0
!
 ! A2    A(2,1,17)              120.7915        -DE/DX =    0.0
!
 ! A3    A(6,1,17)              120.0537        -DE/DX =    0.0
!
 ! A4    A(1,2,3)               121.1065        -DE/DX =    0.0
!
 ! A5    A(1,2,18)              120.771         -DE/DX =    0.0
!
 ! A6    A(3,2,18)              118.1225        -DE/DX =    0.0
!
 ! A7    A(2,3,4)               120.4148        -DE/DX =    0.0
!
 ! A8    A(2,3,7)               120.1178        -DE/DX =    0.0
!
 ! A9    A(4,3,7)               119.4673        -DE/DX =    0.0
!
 ! A10   A(3,4,5)               116.1281        -DE/DX =    0.0
!
 ! A11   A(3,4,8)               119.1826        -DE/DX =    0.0
!
 ! A12   A(5,4,8)               124.6894        -DE/DX =    0.0
!
 ! A13   A(4,5,6)               121.8338        -DE/DX =    0.0
!
 ! A14   A(4,5,19)              120.6569        -DE/DX =    0.0
!
 ! A15   A(6,5,19)              117.5093        -DE/DX =    0.0
!
 ! A16   A(1,6,5)               121.3621        -DE/DX =    0.0
!
 ! A17   A(1,6,20)              119.4448        -DE/DX =    0.0
!
 ! A18   A(5,6,20)              119.1931        -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A19   A(3,7,10)             122.3435         -DE/DX =    0.0
!
 ! A20   A(3,7,16)             118.7883         -DE/DX =    0.0
!
 ! A21   A(10,7,16)            118.8682         -DE/DX =    0.0
!
 ! A22   A(4,8,9)              120.2399         -DE/DX =    0.0
!
 ! A23   A(4,8,24)             118.1613         -DE/DX =    0.0
!
 ! A24   A(9,8,24)             121.5988         -DE/DX =    0.0
!
 ! A25   A(8,9,10)             119.199          -DE/DX =    0.0
!
 ! A26   A(8,9,15)             123.9073         -DE/DX =    0.0
!
 ! A27   A(10,9,15)            116.8937         -DE/DX =    0.0
!
 ! A28   A(7,10,9)             119.5676         -DE/DX =    0.0
!
 ! A29   A(7,10,11)            120.2327         -DE/DX =    0.0
!
 ! A30   A(9,10,11)            120.1997         -DE/DX =    0.0
!
 ! A31   A(10,11,12)           118.2829         -DE/DX =    0.0
!
 ! A32   A(10,11,13)           120.8612         -DE/DX =    0.0
!
 ! A33   A(12,11,13)           120.8559         -DE/DX =    0.0
!
 ! A34   A(11,13,14)           119.3551         -DE/DX =    0.0
!
 ! A35   A(11,13,21)           120.6008         -DE/DX =    0.0
!
 ! A36   A(14,13,21)           120.0441         -DE/DX =    0.0
!
 ! A37   A(13,14,15)           121.5331         -DE/DX =    0.0
!
 ! A38   A(13,14,22)           119.3148         -DE/DX =    0.0
!
 ! A39   A(15,14,22)           119.1522         -DE/DX =    0.0
!
 ! A40   A(9,15,14)            121.1573         -DE/DX =    0.0
!
 ! A41   A(9,15,23)            118.773          -DE/DX =    0.0
!
 ! A42   A(14,15,23)           120.0697         -DE/DX =    0.0
!
 ! A43   A(8,24,25)            115.3437         -DE/DX =    0.0
!
 ! A44   A(8,24,26)            127.3495         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A45   A(25,24,26)           117.3068         -DE/DX =    0.0
!
 ! D1    D(6,1,2,3)             -0.0001         -DE/DX =    0.0
!
 ! D2    D(6,1,2,18)           179.9999         -DE/DX =    0.0
!
 ! D3    D(17,1,2,3)          -180.0            -DE/DX =    0.0
!
 ! D4    D(17,1,2,18)           0.0            -DE/DX =    0.0
!
 ! D5    D(2,1,6,5)             0.0            -DE/DX =    0.0
!
 ! D6    D(2,1,6,20)         -179.9999         -DE/DX =    0.0
!
 ! D7    D(17,1,6,5)           179.9999         -DE/DX =    0.0
!
 ! D8    D(17,1,6,20)           0.0            -DE/DX =    0.0
!
 ! D9    D(1,2,3,4)             0.0            -DE/DX =    0.0
!
 ! D10   D(1,2,3,7)           179.9999         -DE/DX =    0.0
!
 ! D11   D(18,2,3,4)          180.0            -DE/DX =    0.0
!
 ! D12   D(18,2,3,7)            -0.0001         -DE/DX =    0.0
!
 ! D13   D(2,3,4,5)              0.0002         -DE/DX =    0.0
!
 ! D14   D(2,3,4,8)           -180.0001         -DE/DX =    0.0
!
 ! D15   D(7,3,4,5)           -179.9998         -DE/DX =    0.0
!
 ! D16   D(7,3,4,8)             -0.0001         -DE/DX =    0.0
!
 ! D17   D(2,3,7,10)          -179.9999         -DE/DX =    0.0
!
 ! D18   D(2,3,7,16)             0.0            -DE/DX =    0.0
!
 ! D19   D(4,3,7,10)             0.0            -DE/DX =    0.0
!
 ! D20   D(4,3,7,16)           180.0            -DE/DX =    0.0
!
 ! D21   D(3,4,5,6)             -0.0002         -DE/DX =    0.0
!
 ! D22   D(3,4,5,19)           179.9996         -DE/DX =    0.0
!
 ! D23   D(8,4,5,6)            180.0001         -DE/DX =    0.0
!
 ! D24   D(8,4,5,19)             0.0            -DE/DX =    0.0
!
 ! D25   D(3,4,8,9)              0.0001         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D26   D(3,4,8,24)          179.9997         -DE/DX =    0.0
!
 ! D27   D(5,4,8,9)           179.9997         -DE/DX =    0.0
!
 ! D28   D(5,4,8,24)           -0.0007         -DE/DX =    0.0
!
 ! D29   D(4,5,6,1)             0.0001         -DE/DX =    0.0
!
 ! D30   D(4,5,6,20)         -179.9999         -DE/DX =    0.0
!
 ! D31   D(19,5,6,1)         -179.9997         -DE/DX =    0.0
!
 ! D32   D(19,5,6,20)           0.0002         -DE/DX =    0.0
!
 ! D33   D(3,7,10,9)            0.0001         -DE/DX =    0.0
!
 ! D34   D(3,7,10,11)         180.0001         -DE/DX =    0.0
!
 ! D35   D(16,7,10,9)        -179.9999         -DE/DX =    0.0
!
 ! D36   D(16,7,10,11)          0.0002         -DE/DX =    0.0
!
 ! D37   D(4,8,9,10)            0.0            -DE/DX =    0.0
!
 ! D38   D(4,8,9,15)         -180.0003         -DE/DX =    0.0
!
 ! D39   D(24,8,9,10)        -179.9996         -DE/DX =    0.0
!
 ! D40   D(24,8,9,15)           0.0002         -DE/DX =    0.0
!
 ! D41   D(4,8,24,25)           -0.0068         -DE/DX =    0.0
!
 ! D42   D(4,8,24,26)         180.0025         -DE/DX =    0.0
!
 ! D43   D(9,8,24,25)         179.9928         -DE/DX =    0.0
!
 ! D44   D(9,8,24,26)           0.0021         -DE/DX =    0.0
!
 ! D45   D(8,9,10,7)            -0.0001         -DE/DX =    0.0
!
 ! D46   D(8,9,10,11)         179.9999         -DE/DX =    0.0
!
 ! D47   D(15,9,10,7)        -179.9998         -DE/DX =    0.0
!
 ! D48   D(15,9,10,11)          0.0001         -DE/DX =    0.0
!
 ! D49   D(8,9,15,14)        -179.9998         -DE/DX =    0.0
!
 ! D50   D(8,9,15,23)           0.0005         -DE/DX =    0.0
!
 ! D51   D(10,9,15,14)          -0.0001         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D52   D(10,9,15,23)        -179.9997         -DE/DX =    0.0
!
 ! D53   D(7,10,11,12)          -0.0001         -DE/DX =    0.0
!
 ! D54   D(7,10,11,13)         179.9999         -DE/DX =    0.0
!
 ! D55   D(9,10,11,12)         180.0            -DE/DX =    0.0
!
 ! D56   D(9,10,11,13)          -0.0001         -DE/DX =    0.0
!
 ! D57   D(10,11,13,14)         -0.0001         -DE/DX =    0.0
!
 ! D58   D(10,11,13,21)       -180.0            -DE/DX =    0.0
!
 ! D59   D(12,11,13,14)         179.9999         -DE/DX =    0.0
!
 ! D60   D(12,11,13,21)         -0.0001         -DE/DX =    0.0
!
 ! D61   D(11,13,14,15)          0.0001         -DE/DX =    0.0
!
 ! D62   D(11,13,14,22)       -180.0            -DE/DX =    0.0
!
 ! D63   D(21,13,14,15)       -179.9999         -DE/DX =    0.0
!
 ! D64   D(21,13,14,22)          0.0            -DE/DX =    0.0
!
 ! D65   D(13,14,15,9)          -0.0001         -DE/DX =    0.0
!
 ! D66   D(13,14,15,23)         179.9996         -DE/DX =    0.0
!
 ! D67   D(22,14,15,9)          180.0            -DE/DX =    0.0
!
 ! D68   D(22,14,15,23)         -0.0003         -DE/DX =    0.0
!
 ---------------------------------------------------------------------
-----------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -6.634029   -4.463238    0.011133
    2          6             0       -5.266121   -4.409311    0.016037
    3          6             0       -4.575687   -3.155970    0.014867
    4          6             0       -5.315189   -1.912278    0.008430
    5          6             0       -6.746406   -2.027640    0.003477
    6          6             0       -7.375142   -3.249668    0.004782
    7          6             0       -3.178762   -3.125026    0.019949
```

8	6	0	-4.596798	-0.672065	0.007405
9	6	0	-3.165818	-0.668097	0.012694
10	6	0	-2.457255	-1.927786	0.019062
11	6	0	-1.027393	-1.948796	0.024418
12	1	0	-0.526153	-2.914114	0.029143
13	6	0	-0.307320	-0.783053	0.023617
14	6	0	-0.995228	0.460964	0.017369
15	6	0	-2.369873	0.523173	0.012096
16	1	0	-2.633434	-4.067404	0.024771
17	1	0	-7.152999	-5.417697	0.012049
18	1	0	-4.673308	-5.321181	0.020944
19	1	0	-7.371047	-1.144273	-0.001457
20	1	0	-8.461499	-3.286990	0.000872
21	1	0	0.779223	-0.803956	0.027702
22	1	0	-0.423242	1.385512	0.016736
23	1	0	-2.868195	1.481336	0.007407
24	6	0	-5.375145	0.585379	0.000776
25	1	0	-6.470053	0.462295	-0.003038
26	8	0	-4.938011	1.730516	-0.001052

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.368980	0.000000			
3	C	2.438388	1.430930	0.000000		
4	C	2.871714	2.497526	1.446954	0.000000	
5	C	2.438201	2.804239	2.446483	1.435867	0.000000
6	C	1.421985	2.406838	2.801041	2.456019	1.374287
7	C	3.705369	2.450810	1.397277	2.456667	3.732641
8	C	4.303873	3.796719	2.484007	1.433254	2.541341
9	C	5.141166	4.290450	2.859589	2.483506	3.830020
10	C	4.886105	3.748025	2.448715	2.857996	4.290341
11	C	6.144670	4.901124	3.748033	4.287982	5.719595
12	H	6.301290	4.970219	4.056775	4.892747	6.283155
13	C	7.319233	6.143249	4.883623	5.133628	6.558295
14	C	7.486246	6.477662	5.089392	4.928938	6.266529
15	C	6.561046	5.719935	4.289723	3.821822	5.065645
16	H	4.020153	2.654809	2.145496	3.440443	4.591038
17	H	1.086426	2.139432	3.428987	3.957968	3.414363
18	H	2.140231	1.087639	2.167419	3.468831	3.891716
19	H	3.399835	3.884777	3.444014	2.194648	1.081914
20	H	2.173318	3.386780	3.888045	3.433533	2.127795
21	H	8.267220	7.038813	5.848692	6.194401	7.624505
22	H	8.531225	7.552049	6.153687	5.899715	7.185554
23	H	7.037008	6.360019	4.941679	4.183826	5.230052
24	C	5.203214	4.995903	3.825837	2.498389	2.950971
25	H	4.928282	5.018203	4.084212	2.640538	2.505232
26	O	6.421777	6.148611	4.899927	3.662281	4.170618

		6	7	8	9	10
6	C	0.000000				
7	C	4.198258	0.000000			
8	C	3.789886	2.833373	0.000000		

This journal is © The Royal Society of Chemistry 2014

9	C	4.937913	2.456974	1.430996	0.000000	
10	C	5.092463	1.397839	2.480850	1.445309	0.000000
11	C	6.479705	2.451923	3.790908	2.492627	1.430027
12	H	6.857247	2.660997	4.647301	3.465933	2.168433
13	C	7.485897	3.705406	4.290944	2.860829	2.435705
14	C	7.380532	4.198470	3.775601	2.446684	2.800653
15	C	6.267942	3.736806	2.527412	1.432708	2.452527
16	H	4.811744	1.088799	3.922172	3.440766	2.146867
17	H	2.179392	4.588132	5.390288	6.201315	5.850601
18	H	3.404605	2.656458	4.649766	4.891195	4.052903
19	H	2.105408	4.636712	2.814164	4.232127	4.975908
20	H	1.087005	5.285253	4.666239	5.907874	6.156192
21	H	8.513266	4.588362	5.377677	3.947408	3.426056
22	H	8.355475	5.285627	4.653202	3.426230	3.887823
23	H	6.534139	4.616837	2.761377	2.169947	3.433821
24	C	4.325227	4.311794	1.478862	2.540171	3.851028
25	H	3.820722	4.868469	2.189969	3.492278	4.670709
26	O	5.544536	5.164464	2.426704	2.982315	4.420150

		11	12	13	14	15
11	C	0.000000				
12	H	1.087705	0.000000			
13	C	1.370205	2.142275	0.000000		
14	C	2.409985	3.407539	1.421561	0.000000	
15	C	2.813012	3.900582	2.441410	1.376062	0.000000
16	H	2.658547	2.402235	4.024646	4.815589	4.598155
17	H	7.039636	7.084017	8.267005	8.513332	7.627072
18	H	4.966457	4.795095	6.297338	6.852845	6.281908
19	H	6.394519	7.070067	7.073001	6.574816	5.271841
20	H	7.553625	7.944152	8.529997	8.354198	7.185080
21	H	2.138815	2.481285	1.086752	2.179176	3.417356
22	H	3.388609	4.300875	2.171672	1.087179	2.129090
23	H	3.892897	4.980524	3.418450	2.132901	1.080011
24	C	5.032450	5.979965	5.249378	4.381715	3.005937
25	H	5.952870	6.836016	6.287358	5.474863	4.100660
26	O	5.369443	6.406090	5.268959	4.142178	2.837813

		16	17	18	19	20
16	H	0.000000				
17	H	4.716981	0.000000			
18	H	2.394380	2.481584	0.000000		
19	H	5.566898	4.279004	4.972410	0.000000	
20	H	5.880132	2.500442	4.299852	2.404230	0.000000
21	H	4.721899	9.176436	7.080640	8.157424	9.568548
22	H	5.883818	9.569394	7.939951	7.394062	9.297640
23	H	5.553732	8.121343	7.037958	5.212445	7.349967
24	C	5.400551	6.260815	5.948146	2.641085	4.951850
25	H	5.936210	5.919539	6.056192	1.841970	4.245351
26	O	6.239200	7.483535	7.056698	3.766176	6.131096

		21	22	23	24	25
21	H	0.000000				
22	H	2.497962	0.000000			
23	H	4.304257	2.446849	0.000000		
24	C	6.309296	5.016155	2.662251	0.000000	

```
   25  H    7.359099   6.116915   3.743252   1.101811   0.000000
   26  O    6.253890   4.527967   2.084778   1.225736   1.988855
                  26
   26  O    0.000000
 Stoichiometry    C15H10O
 Framework group  C1[X(C15H10O)]
 Deg. of freedom    72
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        3.783424   -0.993997    0.000004
    2          6             0        2.614395   -1.706372    0.000008
    3          6             0        1.345566   -1.044832    0.000003
    4          6             0        1.272909    0.400297   -0.000005
    5          6             0        2.528670    1.096557   -0.000012
    6          6             0        3.728783    0.426937   -0.000006
    7          6             0        0.165096   -1.792410    0.000005
    8          6             0       -0.011936    1.035427   -0.000012
    9          6             0       -1.205833    0.246530   -0.000010
   10          6             0       -1.098553   -1.194792    0.000000
   11          6             0       -2.277692   -2.003871    0.000005
   12          1             0       -2.160720   -3.085269    0.000013
   13          6             0       -3.522710   -1.431690    0.000002
   14          6             0       -3.638514   -0.014854   -0.000005
   15          6             0       -2.528168    0.797967   -0.000011
   16          1             0        0.232652   -2.879111    0.000011
   17          1             0        4.744000   -1.501556    0.000007
   18          1             0        2.625517   -2.793954    0.000014
   19          1             0        2.559833    2.178022   -0.000024
   20          1             0        4.654147    0.997271   -0.000011
   21          1             0       -4.415996   -2.050616    0.000006
   22          1             0       -4.626683    0.438444   -0.000006
   23          1             0       -2.643608    1.871790   -0.000023
   24          6             0       -0.059857    2.513512   -0.000013
   25          1             0        0.920106    3.017159    0.000110
   26          8             0       -1.057840    3.225171    0.000024
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9696461      0.4404288
0.3028634


*********************************************************************

            Population analysis using the SCF density.

*********************************************************************
```

```
 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.14971 -10.27742 -10.23221 -10.22454 -
10.22245
 Alpha  occ. eigenvalues --  -10.22140 -10.21982 -10.21907 -10.21438 -
10.21405
 Alpha  occ. eigenvalues --  -10.21184 -10.21123 -10.20979 -10.20742 -
10.20640
 Alpha  occ. eigenvalues --  -10.19556  -1.04207  -0.90070  -0.86734
-0.82012
 Alpha  occ. eigenvalues --   -0.80869  -0.76807  -0.75792  -0.72861
-0.67261
 Alpha  occ. eigenvalues --   -0.64915  -0.63431  -0.60794  -0.57912
-0.55549
 Alpha  occ. eigenvalues --   -0.54057  -0.51494  -0.48476  -0.48151
-0.47761
 Alpha  occ. eigenvalues --   -0.46500  -0.45335  -0.43090  -0.42854
-0.42574
 Alpha  occ. eigenvalues --   -0.41882  -0.40938  -0.39538  -0.38882
-0.37804
 Alpha  occ. eigenvalues --   -0.36346  -0.35691  -0.35301  -0.32051
-0.31164
 Alpha  occ. eigenvalues --   -0.27286  -0.26015  -0.25326  -0.21750
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --   -0.10049  -0.03947  -0.03523  -0.01564
-0.00149
 Alpha virt. eigenvalues --    0.00535   0.01264   0.02403   0.02410
0.03020
 Alpha virt. eigenvalues --    0.04020   0.04456   0.04682   0.05153
0.05300
 Alpha virt. eigenvalues --    0.06645   0.07078   0.07160   0.07366
0.07548
 Alpha virt. eigenvalues --    0.09037   0.09516   0.09819   0.10763
0.11457
 Alpha virt. eigenvalues --    0.11801   0.11900   0.11941   0.13131
0.13634
 Alpha virt. eigenvalues --    0.13926   0.14104   0.15068   0.15462
0.16713
 Alpha virt. eigenvalues --    0.17210   0.17253   0.17587   0.17763
0.18110
 Alpha virt. eigenvalues --    0.18173   0.18709   0.19194   0.19210
0.19461
 Alpha virt. eigenvalues --    0.19844   0.20081   0.20620   0.21755
0.22564
 Alpha virt. eigenvalues --    0.22580   0.22861   0.23370   0.23982
0.24280
 Alpha virt. eigenvalues --    0.24801   0.25092   0.25265   0.25894
0.26260
 Alpha virt. eigenvalues --    0.26548   0.26964   0.27137   0.28045
0.28724
 Alpha virt. eigenvalues --    0.29198   0.29710   0.30034   0.30720
0.30767
 Alpha virt. eigenvalues --    0.30952   0.31618   0.32123   0.33234
0.33445
 Alpha virt. eigenvalues --    0.35443   0.35784   0.36576   0.37439
0.37812
 Alpha virt. eigenvalues --    0.39292   0.40144   0.41142   0.43728
0.44949
 Alpha virt. eigenvalues --    0.46343   0.48014   0.49215   0.52329
0.56093
 Alpha virt. eigenvalues --    0.58001   0.61431   0.64171   0.64260
0.66302
 Alpha virt. eigenvalues --    0.66673   0.66916   0.67419   0.69739
0.70453
 Alpha virt. eigenvalues --    0.70549   0.71011   0.71016   0.72063
0.72595
 Alpha virt. eigenvalues --    0.73346   0.73370   0.73659   0.74937
0.76113
 Alpha virt. eigenvalues --    0.76287   0.76933   0.77492   0.78089
0.79096
 Alpha virt. eigenvalues --    0.79269   0.79547   0.80808   0.81866
0.85038
 Alpha virt. eigenvalues --    0.87729   0.89256   0.90487   0.91036
0.91096
 Alpha virt. eigenvalues --    0.91851   0.93255   0.95903   0.96402
0.97616
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.99753   1.01381   1.03283   1.05756
1.06988
 Alpha virt. eigenvalues --    1.07497   1.09228   1.11561   1.11706
1.13119
 Alpha virt. eigenvalues --    1.15969   1.17040   1.17528   1.18172
1.18724
 Alpha virt. eigenvalues --    1.19876   1.20209   1.20813   1.21893
1.24322
 Alpha virt. eigenvalues --    1.25960   1.26225   1.28370   1.29415
1.31348
 Alpha virt. eigenvalues --    1.31829   1.33964   1.34851   1.36481
1.39012
 Alpha virt. eigenvalues --    1.41476   1.42752   1.43138   1.45050
1.45296
 Alpha virt. eigenvalues --    1.46894   1.47378   1.47853   1.48233
1.49065
 Alpha virt. eigenvalues --    1.50056   1.51946   1.52798   1.53799
1.54728
 Alpha virt. eigenvalues --    1.62231   1.71304   1.73220   1.74921
1.75754
 Alpha virt. eigenvalues --    1.77974   1.80732   1.81897   1.83787
1.84189
 Alpha virt. eigenvalues --    1.86063   1.90184   1.90951   1.91769
1.93419
 Alpha virt. eigenvalues --    1.93591   1.94161   1.95866   1.97237
1.98504
 Alpha virt. eigenvalues --    1.99288   2.03325   2.03720   2.04924
2.08918
 Alpha virt. eigenvalues --    2.09386   2.10613   2.14820   2.15496
2.17243
 Alpha virt. eigenvalues --    2.19181   2.20500   2.22888   2.25522
2.25671
 Alpha virt. eigenvalues --    2.25921   2.29342   2.29761   2.30853
2.34772
 Alpha virt. eigenvalues --    2.36747   2.39583   2.40053   2.44452
2.46619
 Alpha virt. eigenvalues --    2.51557   2.54020   2.54173   2.59353
2.61384
 Alpha virt. eigenvalues --    2.64202   2.66794   2.67321   2.68007
2.69077
 Alpha virt. eigenvalues --    2.71714   2.72596   2.74511   2.75918
2.82319
 Alpha virt. eigenvalues --    2.84849   2.85416   2.88921   2.93175
2.95024
 Alpha virt. eigenvalues --    3.00263   3.11574   3.13495   3.22494
3.28190
 Alpha virt. eigenvalues --    3.44205   3.46709   4.19565   4.20880
4.23102
 Alpha virt. eigenvalues --    4.24669   4.28447   4.29623   4.31865
4.32888
 Alpha virt. eigenvalues --    4.36830   4.41178   4.41803   4.44643
4.48504
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    4.53753   4.66817   4.85976
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C    6.125702   0.191819  -0.514099   0.223411  -0.877888
1.088918
     2  C    0.191819   7.538793  -0.534423  -0.533138   1.585773  -
1.263142
     3  C   -0.514099  -0.534423   7.938662  -0.681780   1.350424  -
0.600809
     4  C    0.223411  -0.533138  -0.681780   9.914571  -3.444469
1.416354
     5  C   -0.877888   1.585773   1.350424  -3.444469  12.094943  -
3.220462
     6  C    1.088918  -1.263142  -0.600809   1.416354  -3.220462
8.388462
     7  C   -0.036100  -0.514144   0.824523  -1.013171   0.544241  -
0.277118
     8  C    0.006418  -0.299879  -0.166015   1.085289  -1.242953
0.276646
     9  C   -0.022202  -0.091519  -0.495350  -0.266343  -0.375201
0.121998
    10  C   -0.007317   0.012153  -0.747071  -0.729280  -0.114763  -
0.056744
    11  C   -0.037670  -0.204597   0.012934  -0.059399  -0.195501
0.023699
    12  H    0.000610   0.004365  -0.006295  -0.000590   0.000058  -
0.000072
    13  C    0.016051  -0.060618  -0.027079  -0.031982  -0.063363
0.012428
    14  C    0.000020   0.029010   0.091157   0.215672   0.120822  -
0.038082
    15  C   -0.055617  -0.080987  -0.137119  -0.262318  -0.169155
0.057883
    16  H   -0.005156  -0.003637  -0.061729   0.000714   0.003127
0.001384
    17  H    0.287229   0.000500   0.003533   0.014811   0.015478  -
0.015233
    18  H    0.015758   0.266932  -0.054000   0.062644  -0.037953
0.013165
    19  H    0.002584  -0.029863   0.012613  -0.000762   0.256409  -
0.011324
    20  H   -0.009520   0.013572   0.009947  -0.014236   0.008668
0.293937
    21  H    0.000012   0.000151  -0.001389  -0.000103  -0.000019  -
0.000006
    22  H    0.000000  -0.000036   0.000278  -0.000750  -0.000032
0.000007
    23  H   -0.000114  -0.000272   0.000030   0.008164   0.002777
0.000420
    24  C   -0.000022   0.127132  -0.385674  -0.110451   0.309778  -
0.044103
```

This journal is © The Royal Society of Chemistry 2014

25	H	0.002030	0.000178	-0.048708	-0.006631	0.016915	0.031257
26	O	0.000667	-0.006493	-0.016033	-0.007085	0.022296	0.011977

		7	8	9	10	11	12
1	C	-0.036100	0.006418	-0.022202	-0.007317	-0.037670	0.000610
2	C	-0.514144	-0.299879	-0.091519	0.012153	-0.204597	0.004365
3	C	0.824523	-0.166015	-0.495350	-0.747071	0.012934	-0.006295
4	C	-1.013171	1.085289	-0.266343	-0.729280	-0.059399	-0.000590
5	C	0.544241	-1.242953	-0.375201	-0.114763	-0.195501	0.000058
6	C	-0.277118	0.276646	0.121998	-0.056744	0.023699	-0.000072
7	C	6.763450	-0.204249	-0.842098	0.557958	-0.310195	0.003380
8	C	-0.204249	6.882388	1.086094	-0.037878	-0.165966	0.003711
9	C	-0.842098	1.086094	10.145123	-0.266857	-0.588881	0.056338
10	C	0.557958	-0.037878	-0.266857	7.674617	-0.287332	-0.050075
11	C	-0.310195	-0.165966	-0.588881	-0.287332	6.945205	0.278261
12	H	0.003380	0.003711	0.056338	-0.050075	0.278261	0.538438
13	C	0.042629	-0.012856	0.210227	-0.629613	0.483719	0.012219
14	C	-0.355382	0.204315	0.879205	-0.110243	-0.929642	0.012522
15	C	0.625705	-0.873235	-3.605804	1.061389	1.185462	-0.036656
16	H	0.345292	-0.004420	0.016262	-0.035280	0.007996	0.004392
17	H	-0.008685	0.000530	0.000217	-0.001757	0.000018	0.000000
18	H	0.003541	0.005261	0.000057	-0.005086	0.006494	0.000003
19	H	0.002813	0.051704	0.008267	0.004289	0.000317	0.000000
20	H	0.001949	-0.006260	-0.000845	0.000726	-0.000014	0.000000
21	H	-0.008871	0.002376	0.025773	-0.005143	-0.012369	-0.004319
22	H	0.000503	-0.005354	0.008090	-0.003930	0.011660	-0.000169
23	H	0.001731	-0.001654	-0.126587	0.047469	-0.017540	0.000015

This journal is © The Royal Society of Chemistry 2014

24	C	-0.064356	-0.544791	-0.490879	-0.350792	-0.038425	-0.000126
25	H	-0.001636	-0.195713	-0.005672	-0.012863	-0.002827	0.000000
26	O	0.016741	-0.065724	-0.057948	0.002385	-0.018362	-0.000002

		13	14	15	16	17	18
1	C	0.016051	0.000020	-0.055617	-0.005156	0.287229	0.015758
2	C	-0.060618	0.029010	-0.080987	-0.003637	0.000500	0.266932
3	C	-0.027079	0.091157	-0.137119	-0.061729	0.003533	-0.054000
4	C	-0.031982	0.215672	-0.262318	0.000714	0.014811	0.062644
5	C	-0.063363	0.120822	-0.169155	0.003127	0.015478	-0.037953
6	C	0.012428	-0.038082	0.057883	0.001384	-0.015233	0.013165
7	C	0.042629	-0.355382	0.625705	0.345292	-0.008685	0.003541
8	C	-0.012856	0.204315	-0.873235	-0.004420	0.000530	0.005261
9	C	0.210227	0.879205	-3.605804	0.016262	0.000217	0.000057
10	C	-0.629613	-0.110243	1.061389	-0.035280	-0.001757	-0.005086
11	C	0.483719	-0.929642	1.185462	0.007996	0.000018	0.006494
12	H	0.012219	0.012522	-0.036656	0.004392	0.000000	0.000003
13	C	6.050153	0.728426	-0.571431	-0.002574	0.000000	0.000910
14	C	0.728426	8.314722	-3.021273	0.003207	0.000002	-0.000137
15	C	-0.571431	-3.021273	12.012243	0.003635	0.000022	0.000072
16	H	-0.002574	0.003207	0.003635	0.530662	-0.000014	0.004479
17	H	0.000000	0.000002	0.000022	-0.000014	0.524900	-0.004327
18	H	0.000910	-0.000137	0.000072	0.004479	-0.004327	0.536641
19	H	0.000103	-0.000470	-0.000350	0.000002	-0.000179	0.000018
20	H	-0.000001	0.000004	-0.000092	0.000000	-0.003777	-0.000169
21	H	0.287044	-0.019612	0.028738	-0.000014	0.000000	0.000000
22	H	-0.017518	0.303944	0.000366	0.000000	0.000000	0.000000

This journal is © The Royal Society of Chemistry 2014

23	H	0.012226	0.084196	0.316841	0.000001	0.000000	0.000000
24	C	-0.054717	-0.061754	0.031409	0.001081	0.000455	-0.000241
25	H	-0.000184	-0.003134	-0.015357	0.000000	0.000000	0.000000
26	O	-0.010687	-0.000314	-0.020493	-0.000002	0.000000	0.000000

		19	20	21	22	23	24
1	C	0.002584	-0.009520	0.000012	0.000000	-0.000114	-0.000022
2	C	-0.029863	0.013572	0.000151	-0.000036	-0.000272	0.127132
3	C	0.012613	0.009947	-0.001389	0.000278	0.000030	-0.385674
4	C	-0.000762	-0.014236	-0.000103	-0.000750	0.008164	-0.110451
5	C	0.256409	0.008668	-0.000019	-0.000032	0.002777	0.309778
6	C	-0.011324	0.293937	-0.000006	0.000007	0.000420	-0.044103
7	C	0.002813	0.001949	-0.008871	0.000503	0.001731	-0.064356
8	C	0.051704	-0.006260	0.002376	-0.005354	-0.001654	-0.544791
9	C	0.008267	-0.000845	0.025773	0.008090	-0.126587	-0.490879
10	C	0.004289	0.000726	-0.005143	-0.003930	0.047469	-0.350792
11	C	0.000317	-0.000014	-0.012369	0.011660	-0.017540	-0.038425
12	H	0.000000	0.000000	-0.004319	-0.000169	0.000015	-0.000126
13	C	0.000103	-0.000001	0.287044	-0.017518	0.012226	-0.054717
14	C	-0.000470	0.000004	-0.019612	0.303944	0.084196	-0.061754
15	C	-0.000350	-0.000092	0.028738	0.000366	0.316841	0.031409
16	H	0.000002	0.000000	-0.000014	0.000000	0.000001	0.001081
17	H	-0.000179	-0.003777	0.000000	0.000000	0.000000	0.000455
18	H	0.000018	-0.000169	0.000000	0.000000	0.000000	-0.000241
19	H	0.542994	-0.005390	0.000000	0.000000	-0.000001	-0.022604
20	H	-0.005390	0.527478	0.000000	0.000000	0.000000	-0.001207
21	H	0.000000	0.000000	0.526322	-0.003772	-0.000150	0.000398

This journal is © The Royal Society of Chemistry 2014

```
    22  H    0.000000   0.000000  -0.003772   0.525859  -0.004517  -
0.001464
    23  H   -0.000001   0.000000  -0.000150  -0.004517   0.466425  -
0.029258
    24  C   -0.022604  -0.001207   0.000398  -0.001464  -0.029258
6.951488
    25  H    0.004768   0.000017   0.000000   0.000000  -0.000043
0.517509
    26  O    0.001549   0.000001   0.000011   0.000272  -0.012035
0.360485
              25         26
     1  C    0.002030   0.000667
     2  C    0.000178  -0.006493
     3  C   -0.048708  -0.016033
     4  C   -0.006631  -0.007085
     5  C    0.016915   0.022296
     6  C    0.031257   0.011977
     7  C   -0.001636   0.016741
     8  C   -0.195713  -0.065724
     9  C   -0.005672  -0.057948
    10  C   -0.012863   0.002385
    11  C   -0.002827  -0.018362
    12  H    0.000000  -0.000002
    13  C   -0.000184  -0.010687
    14  C   -0.003134  -0.000314
    15  C   -0.015357  -0.020493
    16  H    0.000000  -0.000002
    17  H    0.000000   0.000000
    18  H    0.000000   0.000000
    19  H    0.004768   0.001549
    20  H    0.000017   0.000001
    21  H    0.000000   0.000011
    22  H    0.000000   0.000272
    23  H   -0.000043  -0.012035
    24  C    0.517509   0.360485
    25  H    0.647212  -0.070031
    26  O   -0.070031   8.272288
 Mulliken atomic charges:
              1
     1  C   -0.395526
     2  C   -0.147629
     3  C    0.233472
     4  C    0.220858
     5  C   -0.589948
     6  C   -0.211440
     7  C   -0.098451
     8  C    0.222215
     9  C    0.678537
    10  C    0.091039
    11  C   -0.087046
    12  H    0.183991
    13  C   -0.373510
```

This journal is © The Royal Society of Chemistry 2014

```
   14  C   -0.447180
   15  C   -0.473878
   16  H    0.190591
   17  H    0.186277
   18  H    0.185937
   19  H    0.182514
   20  H    0.185213
   21  H    0.184940
   22  H    0.186563
   23  H    0.251878
   24  C   -0.098872
   25  H    0.142913
   26  O   -0.403460
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  C   -0.209249
    2  C    0.038309
    3  C    0.233472
    4  C    0.220858
    5  C   -0.407434
    6  C   -0.026226
    7  C    0.092140
    8  C    0.222215
    9  C    0.678537
   10  C    0.091039
   11  C    0.096945
   12  H    0.000000
   13  C   -0.188570
   14  C   -0.260617
   15  C   -0.222000
   16  H    0.000000
   17  H    0.000000
   18  H    0.000000
   19  H    0.000000
   20  H    0.000000
   21  H    0.000000
   22  H    0.000000
   23  H    0.000000
   24  C    0.044041
   25  H    0.000000
   26  O   -0.403460
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  3467.5231
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     1.8401    Y=    -3.4664    Z=     0.0000  Tot=     3.9245
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=   -78.5688   YY=   -93.7908   ZZ=   -98.4751
  XY=     6.8886   XZ=     0.0001   YZ=    -0.0002
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    11.7094   YY=    -3.5125   ZZ=    -8.1969
```

XY= 6.8886 XZ= 0.0001 YZ= -0.0002
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= -0.2518 YYY= -51.9574 ZZZ= 0.0002 XYY= 24.1607
XXY= -5.8195 XXZ= 0.0000 XZZ= -2.3790 YZZ= 8.7664
YYZ= -0.0002 XYZ= 0.0002
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -2854.2892 YYYY= -1560.8320 ZZZZ= -117.8654 XXXY= 4.1954
XXXZ= -0.0003 YYYX= 77.3566 YYYZ= -0.0017 ZZZX= -0.0002
ZZZY= 0.0005 XXYY= -741.3321 XXZZ= -630.0252 YYZZ= -278.7375
XXYZ= -0.0007 YYXZ= 0.0009 ZZXY= -7.0909
N-N= 9.633251563010D+02 E-N=-3.440040593294D+03 KE=
6.465764680046D+02
1\1\GINC-OPT0195\FOpt\RB3LYP\6-31+G(d)\C15H10O1\UCN0868\03-Nov-
2011\0\
\# opt rb3lyp/6-31+g(d)
geom=connectivity\\aldehydeanthracene\\0,1\C,-
6.6340293788,-4.463238045,0.0111327069\C,-5.2661206488,-
4.4093105906,0
.0160371345\C,-4.5756870572,-3.1559704898,0.0148668558\C,-
5.3151894147
,-1.9122783127,0.0084297707\C,-6.7464059303,-
2.0276398607,0.0034767725
\C,-7.3751421007,-3.2496680397,0.0047815164\C,-3.1787621556,-
3.1250259
277,0.0199489714\C,-4.5967983749,-0.6720648086,0.0074052817\C,-
3.16581
79013,-0.6680971204,0.0126938911\C,-2.4572554007,-
1.9277864922,0.01906
20064\C,-1.0273929616,-1.9487960136,0.0244180025\H,-0.5261532018,-
2.91
4114186,0.029143487\C,-0.3073202185,-0.7830528099,0.0236169216\C,-
0.99
52281238,0.4609641009,0.0173688978\C,-
2.369873234,0.5231730405,0.01209
60285\H,-2.6334344497,-4.0674044606,0.0247713508\H,-7.1529989298,-
5.41
7696647,0.012049399\H,-4.6733080919,-5.3211811853,0.0209440131\H,-
7.37
10472847,-1.1442733514,-0.0014572957\H,-8.4614988161,-
3.2869897653,0.0
008718101\H,0.7792226232,-0.8039564032,0.0277018907\H,-
0.4232417037,1.
3855119916,0.0167361362\H,-2.8681953736,1.4813361204,0.0074067307\C,-
5
.3751449129,0.5853790059,0.000775775\H,-6.470052966,0.4622948724,-
0.00
30382605\O,-4.9380106937,1.7305162295,-0.0010520404\\Version=AM64L-
G03
RevD.01\State=1-A\HF=-652.8680473\RMSD=5.591e-09\RMSF=3.173e-
05\Therma
l=0.\Dipole=0.1520885,-1.5364855,0.0051492\PG=C01 [X(C15H10O1)]\\@

This journal is © The Royal Society of Chemistry 2014

```
 Sometimes the fool who rushes in gets the job done.
                                       -- Al Bernstein
 Job cpu time:  0 days  5 hours 25 minutes 51.5 seconds.
 File lengths (MBytes):  RWF=     79 Int=      0 D2E=      0 Chk=
13 Scr=      1
 Normal termination of Gaussian 03 at Thu Nov  3 01:52:42 2011.
```

This journal is © The Royal Society of Chemistry 2014

Transition State of Maleic anhydride and 9-formyl anthracene

```
Entering Gaussian System, Link 0=g03
 Initial command:
 /usr/local/g03d01/g03/l1.exe /tmp/pbstmp.6601740/Gau-18723.inp -
scrdir=/tmp/pbstmp.6601740/
 Entering Link 1 = /usr/local/g03d01/g03/l1.exe PID=     18724.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2004, Gaussian, Inc.
                    All Rights Reserved.

 This is the Gaussian(R) 03 program.  It is based on the
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,
 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be
 used, copied, transmitted, or stored only in accord with that
 written license.

 The following legend is applicable only to US Government
 contracts under FAR:

                       RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is
 subject to restrictions as set forth in subparagraphs (a)
 and (c) of the Commercial Computer Software - Restricted
 Rights clause in FAR 52.227-19.

 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ----------------------------------------------------------------------
 Warning -- This program may not be used in any manner that
 competes with the business of Gaussian, Inc. or will provide
 assistance to any competitor of Gaussian, Inc.  The licensee
 of this program is prohibited from giving any competitor of
 Gaussian, Inc. access to this program.  By using this program,
 the user acknowledges that Gaussian, Inc. is engaged in the
 business of creating and licensing software in the field of
 computational chemistry and represents and warrants to the
```

This journal is © The Royal Society of Chemistry 2014

```
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.
----------------------------------------------------------------


Cite this work as:
Gaussian 03, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

******************************************
Gaussian 03:  AM64L-G03RevD.01 13-Oct-2005
                4-Nov-2011
******************************************
%chk=daant.chk
%mem=450MW
%nprocshared=4
Will use up to    4 processors via shared memory.
----------------------------------------------------
# opt=(calcfc,ts) b3lyp/6-31+g(d) geom=connectivity
----------------------------------------------------
1/5=1,10=4,14=-1,18=20,26=3,38=1,57=2/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,7=6/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/10=1,18=20,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20/3(3);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99//99;
2/9=110/2;
```

This journal is © The Royal Society of Chemistry 2014

```
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4/5=5,16=3/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/5=1,14=-1,18=20/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
---------------------
Title Card Required
---------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                    -0.57989   0.49011   1.14087
C                     0.56322   1.03473   0.42466
C                    -0.74236  -0.92322   1.09257
C                     0.24322  -1.66302   0.34936
H                     0.08327  -2.73402   0.23255
C                    -0.20053  -0.93802  -1.65298
H                     0.49935  -1.62135  -2.11665
C                    -0.06113   0.46793  -1.62931
H                     0.76289   1.02022  -2.06156
C                    -1.57266   1.26302   1.78917
H                    -1.48595   2.34306   1.83422
C                    -2.65867   0.64651   2.38912
H                    -3.40165   1.25127   2.90173
C                    -2.81686  -0.75274   2.33041
H                    -3.68054  -1.21998   2.79508
C                    -1.87896  -1.52849   1.67249
H                    -2.00103  -2.60628   1.60373
C                     1.60157  -1.17939   0.3533
C                     1.77596   0.23026   0.38424
C                     3.0817    0.76032   0.27912
H                     3.21414   1.83611   0.27818
C                     4.17345  -0.09013   0.1863
H                     5.17556   0.32678   0.1323
C                     3.99605  -1.48835   0.15431
H                     4.86027  -2.14264   0.07716
C                     2.72129  -2.02751   0.21862
H                     2.57423  -3.10463   0.18507
C                    -1.4298    1.03759  -1.69821
C                    -1.65102  -1.2304   -1.74909
O                    -2.34323  -0.02014  -1.6555
O                    -2.22676  -2.27958  -1.87135
O                    -1.79583   2.18151  -1.7671
C                     0.68031   2.53117   0.29209
H                    -0.12597   3.13928   0.70176
O                     1.62282   3.07696  -0.27177
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Initialization pass.
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
 --------------------------                           ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ------------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.4547         calculate D2E/DX2
analytically  !
 ! R2    R(1,3)                  1.4235         calculate D2E/DX2
analytically  !
 ! R3    R(1,8)                  2.8184         calculate D2E/DX2
analytically  !
 ! R4    R(1,10)                 1.4154         calculate D2E/DX2
analytically  !
 ! R5    R(2,8)                  2.2203         calculate D2E/DX2
analytically  !
 ! R6    R(2,9)                  2.4943         calculate D2E/DX2
analytically  !
 ! R7    R(2,19)                 1.4559         calculate D2E/DX2
analytically  !
 ! R8    R(2,33)                 1.5069         calculate D2E/DX2
analytically  !
 ! R9    R(3,4)                  1.4391         calculate D2E/DX2
analytically  !
 ! R10   R(3,6)                  2.7985         calculate D2E/DX2
analytically  !
 ! R11   R(3,16)                 1.4123         calculate D2E/DX2
analytically  !
 ! R12   R(4,5)                  1.0892         calculate D2E/DX2
analytically  !
 ! R13   R(4,6)                  2.1753         calculate D2E/DX2
analytically  !
 ! R14   R(4,7)                  2.4796         calculate D2E/DX2
analytically  !
 ! R15   R(4,18)                 1.4419         calculate D2E/DX2
analytically  !
 ! R16   R(5,6)                  2.6194         calculate D2E/DX2
analytically  !
 ! R17   R(6,7)                  1.0825         calculate D2E/DX2
analytically  !
 ! R18   R(6,8)                  1.413          calculate D2E/DX2
analytically  !
 ! R19   R(6,18)                 2.7076         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R20   R(6,29)                 1.4828         calculate D2E/DX2
analytically  !
 ! R21   R(7,18)                 2.7406         calculate D2E/DX2
analytically  !
 ! R22   R(8,9)                  1.0821         calculate D2E/DX2
analytically  !
 ! R23   R(8,19)                 2.736          calculate D2E/DX2
analytically  !
 ! R24   R(8,28)                 1.4841         calculate D2E/DX2
analytically  !
 ! R25   R(9,19)                 2.7627         calculate D2E/DX2
analytically  !
 ! R26   R(9,33)                 2.7981         calculate D2E/DX2
analytically  !
 ! R27   R(10,11)                1.0845         calculate D2E/DX2
analytically  !
 ! R28   R(10,12)                1.3854         calculate D2E/DX2
analytically  !
 ! R29   R(12,13)                1.0865         calculate D2E/DX2
analytically  !
 ! R30   R(12,14)                1.4094         calculate D2E/DX2
analytically  !
 ! R31   R(14,15)                1.0864         calculate D2E/DX2
analytically  !
 ! R32   R(14,16)                1.3836         calculate D2E/DX2
analytically  !
 ! R33   R(16,17)                1.0869         calculate D2E/DX2
analytically  !
 ! R34   R(18,19)                1.4207         calculate D2E/DX2
analytically  !
 ! R35   R(18,26)                1.4111         calculate D2E/DX2
analytically  !
 ! R36   R(19,20)                1.4131         calculate D2E/DX2
analytically  !
 ! R37   R(20,21)                1.0839         calculate D2E/DX2
analytically  !
 ! R38   R(20,22)                1.387          calculate D2E/DX2
analytically  !
 ! R39   R(21,35)                2.0915         calculate D2E/DX2
analytically  !
 ! R40   R(22,23)                1.0867         calculate D2E/DX2
analytically  !
 ! R41   R(22,24)                1.4098         calculate D2E/DX2
analytically  !
 ! R42   R(24,25)                1.0867         calculate D2E/DX2
analytically  !
 ! R43   R(24,26)                1.3856         calculate D2E/DX2
analytically  !
 ! R44   R(26,27)                1.0876         calculate D2E/DX2
analytically  !
 ! R45   R(28,30)                1.3982         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R46   R(28,32)              1.203          calculate D2E/DX2
analytically  !
 ! R47   R(29,30)              1.3974         calculate D2E/DX2
analytically  !
 ! R48   R(29,31)              1.203          calculate D2E/DX2
analytically  !
 ! R49   R(33,34)              1.0898         calculate D2E/DX2
analytically  !
 ! R50   R(33,35)              1.2264         calculate D2E/DX2
analytically  !
 ! A1    A(2,1,3)             116.4035         calculate D2E/DX2
analytically  !
 ! A2    A(2,1,10)            124.9062         calculate D2E/DX2
analytically  !
 ! A3    A(3,1,10)            118.5342         calculate D2E/DX2
analytically  !
 ! A4    A(1,2,19)            117.4751         calculate D2E/DX2
analytically  !
 ! A5    A(1,2,33)            118.4349         calculate D2E/DX2
analytically  !
 ! A6    A(19,2,33)           118.7885         calculate D2E/DX2
analytically  !
 ! A7    A(1,3,4)             116.7288         calculate D2E/DX2
analytically  !
 ! A8    A(1,3,16)            120.2287         calculate D2E/DX2
analytically  !
 ! A9    A(4,3,16)            122.8825         calculate D2E/DX2
analytically  !
 ! A10   A(3,4,5)             117.407          calculate D2E/DX2
analytically  !
 ! A11   A(3,4,18)            118.1212         calculate D2E/DX2
analytically  !
 ! A12   A(5,4,18)            117.935          calculate D2E/DX2
analytically  !
 ! A13   A(7,6,8)             124.8543         calculate D2E/DX2
analytically  !
 ! A14   A(7,6,29)            118.7006         calculate D2E/DX2
analytically  !
 ! A15   A(8,6,29)            107.0845         calculate D2E/DX2
analytically  !
 ! A16   A(6,8,9)             125.1887         calculate D2E/DX2
analytically  !
 ! A17   A(6,8,28)            106.8677         calculate D2E/DX2
analytically  !
 ! A18   A(9,8,28)            119.1986         calculate D2E/DX2
analytically  !
 ! A19   A(1,10,11)           120.4517         calculate D2E/DX2
analytically  !
 ! A20   A(1,10,12)           120.3431         calculate D2E/DX2
analytically  !
 ! A21   A(11,10,12)          119.2            calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A22   A(10,12,13)          119.5153         calculate D2E/DX2
analytically  !
 ! A23   A(10,12,14)          120.7788         calculate D2E/DX2
analytically  !
 ! A24   A(13,12,14)          119.7029         calculate D2E/DX2
analytically  !
 ! A25   A(12,14,15)          119.8953         calculate D2E/DX2
analytically  !
 ! A26   A(12,14,16)          120.0253         calculate D2E/DX2
analytically  !
 ! A27   A(15,14,16)          120.0773         calculate D2E/DX2
analytically  !
 ! A28   A(3,16,14)           120.0342         calculate D2E/DX2
analytically  !
 ! A29   A(3,16,17)           119.3021         calculate D2E/DX2
analytically  !
 ! A30   A(14,16,17)          120.661          calculate D2E/DX2
analytically  !
 ! A31   A(4,18,19)           116.6473         calculate D2E/DX2
analytically  !
 ! A32   A(4,18,26)           123.0706         calculate D2E/DX2
analytically  !
 ! A33   A(19,18,26)          120.0679         calculate D2E/DX2
analytically  !
 ! A34   A(2,19,18)           116.5269         calculate D2E/DX2
analytically  !
 ! A35   A(2,19,20)           124.3675         calculate D2E/DX2
analytically  !
 ! A36   A(18,19,20)          118.9442         calculate D2E/DX2
analytically  !
 ! A37   A(19,20,21)          119.0282         calculate D2E/DX2
analytically  !
 ! A38   A(19,20,22)          120.1521         calculate D2E/DX2
analytically  !
 ! A39   A(21,20,22)          120.8188         calculate D2E/DX2
analytically  !
 ! A40   A(20,22,23)          119.5996         calculate D2E/DX2
analytically  !
 ! A41   A(20,22,24)          120.7028         calculate D2E/DX2
analytically  !
 ! A42   A(23,22,24)          119.6968         calculate D2E/DX2
analytically  !
 ! A43   A(22,24,25)          119.9126         calculate D2E/DX2
analytically  !
 ! A44   A(22,24,26)          120.0428         calculate D2E/DX2
analytically  !
 ! A45   A(25,24,26)          120.0445         calculate D2E/DX2
analytically  !
 ! A46   A(18,26,24)          120.0392         calculate D2E/DX2
analytically  !
 ! A47   A(18,26,27)          119.3982         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A48   A(24,26,27)          120.5525         calculate D2E/DX2
analytically  !
 ! A49   A(8,28,30)           108.1007         calculate D2E/DX2
analytically  !
 ! A50   A(8,28,32)           130.409          calculate D2E/DX2
analytically  !
 ! A51   A(30,28,32)          121.4869         calculate D2E/DX2
analytically  !
 ! A52   A(6,29,30)           108.0265         calculate D2E/DX2
analytically  !
 ! A53   A(6,29,31)           130.295          calculate D2E/DX2
analytically  !
 ! A54   A(30,29,31)          121.6742         calculate D2E/DX2
analytically  !
 ! A55   A(28,30,29)          109.2405         calculate D2E/DX2
analytically  !
 ! A56   A(2,33,34)           117.6178         calculate D2E/DX2
analytically  !
 ! A57   A(2,33,35)           122.8274         calculate D2E/DX2
analytically  !
 ! A58   A(34,33,35)          119.5418         calculate D2E/DX2
analytically  !
 ! D1    D(3,1,2,19)          -33.8889         calculate D2E/DX2
analytically  !
 ! D2    D(3,1,2,33)          172.1042         calculate D2E/DX2
analytically  !
 ! D3    D(10,1,2,19)         150.7378         calculate D2E/DX2
analytically  !
 ! D4    D(10,1,2,33)          -3.2692         calculate D2E/DX2
analytically  !
 ! D5    D(2,1,3,4)             0.3743         calculate D2E/DX2
analytically  !
 ! D6    D(2,1,3,16)         -175.1599         calculate D2E/DX2
analytically  !
 ! D7    D(10,1,3,4)          176.056          calculate D2E/DX2
analytically  !
 ! D8    D(10,1,3,16)           0.5219         calculate D2E/DX2
analytically  !
 ! D9    D(2,1,10,11)          -4.0077         calculate D2E/DX2
analytically  !
 ! D10   D(2,1,10,12)          176.8297         calculate D2E/DX2
analytically  !
 ! D11   D(3,1,10,11)         -179.2905         calculate D2E/DX2
analytically  !
 ! D12   D(3,1,10,12)            1.5469         calculate D2E/DX2
analytically  !
 ! D13   D(1,2,19,18)           33.3311         calculate D2E/DX2
analytically  !
 ! D14   D(1,2,19,20)         -151.3495         calculate D2E/DX2
analytically  !
 ! D15   D(33,2,19,18)        -172.7562         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D16   D(33,2,19,20)          2.5632         calculate D2E/DX2
analytically  !
 ! D17   D(1,2,33,34)           -2.7752         calculate D2E/DX2
analytically  !
 ! D18   D(1,2,33,35)          178.5442         calculate D2E/DX2
analytically  !
 ! D19   D(19,2,33,34)        -156.4371         calculate D2E/DX2
analytically  !
 ! D20   D(19,2,33,35)          24.8823         calculate D2E/DX2
analytically  !
 ! D21   D(1,3,4,5)           -174.8522         calculate D2E/DX2
analytically  !
 ! D22   D(1,3,4,18)            34.0514         calculate D2E/DX2
analytically  !
 ! D23   D(16,3,4,5)             0.5528         calculate D2E/DX2
analytically  !
 ! D24   D(16,3,4,18)         -150.5436         calculate D2E/DX2
analytically  !
 ! D25   D(1,3,16,14)           -2.2132         calculate D2E/DX2
analytically  !
 ! D26   D(1,3,16,17)          178.3786         calculate D2E/DX2
analytically  !
 ! D27   D(4,3,16,14)         -177.463          calculate D2E/DX2
analytically  !
 ! D28   D(4,3,16,17)            3.1288         calculate D2E/DX2
analytically  !
 ! D29   D(3,4,18,19)          -34.6285         calculate D2E/DX2
analytically  !
 ! D30   D(3,4,18,26)          150.6967         calculate D2E/DX2
analytically  !
 ! D31   D(5,4,18,19)          174.4285         calculate D2E/DX2
analytically  !
 ! D32   D(5,4,18,26)           -0.2463         calculate D2E/DX2
analytically  !
 ! D33   D(7,6,8,9)             -0.6448         calculate D2E/DX2
analytically  !
 ! D34   D(7,6,8,28)           146.2382         calculate D2E/DX2
analytically  !
 ! D35   D(29,6,8,9)          -146.3627         calculate D2E/DX2
analytically  !
 ! D36   D(29,6,8,28)            0.5202         calculate D2E/DX2
analytically  !
 ! D37   D(7,6,29,30)         -153.5991         calculate D2E/DX2
analytically  !
 ! D38   D(7,6,29,31)           27.1629         calculate D2E/DX2
analytically  !
 ! D39   D(8,6,29,30)           -5.3996         calculate D2E/DX2
analytically  !
 ! D40   D(8,6,29,31)          175.3623         calculate D2E/DX2
analytically  !
 ! D41   D(6,8,28,30)            4.5265         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D42   D(6,8,28,32)         -176.1417         calculate D2E/DX2
analytically  !
 ! D43   D(9,8,28,30)          153.7624         calculate D2E/DX2
analytically  !
 ! D44   D(9,8,28,32)          -26.9058         calculate D2E/DX2
analytically  !
 ! D45   D(1,10,12,13)         178.6766         calculate D2E/DX2
analytically  !
 ! D46   D(1,10,12,14)          -1.9592         calculate D2E/DX2
analytically  !
 ! D47   D(11,10,12,13)         -0.4964         calculate D2E/DX2
analytically  !
 ! D48   D(11,10,12,14)        178.8678         calculate D2E/DX2
analytically  !
 ! D49   D(10,12,14,15)       -179.225          calculate D2E/DX2
analytically  !
 ! D50   D(10,12,14,16)          0.2499         calculate D2E/DX2
analytically  !
 ! D51   D(13,12,14,15)          0.1381         calculate D2E/DX2
analytically  !
 ! D52   D(13,12,14,16)        179.6129         calculate D2E/DX2
analytically  !
 ! D53   D(12,14,16,3)           1.8332         calculate D2E/DX2
analytically  !
 ! D54   D(12,14,16,17)       -178.7668         calculate D2E/DX2
analytically  !
 ! D55   D(15,14,16,3)        -178.693          calculate D2E/DX2
analytically  !
 ! D56   D(15,14,16,17)          0.7071         calculate D2E/DX2
analytically  !
 ! D57   D(4,18,19,2)            0.7047         calculate D2E/DX2
analytically  !
 ! D58   D(4,18,19,20)        -174.8808         calculate D2E/DX2
analytically  !
 ! D59   D(26,18,19,2)         175.5488         calculate D2E/DX2
analytically  !
 ! D60   D(26,18,19,20)         -0.0367         calculate D2E/DX2
analytically  !
 ! D61   D(4,18,26,24)         176.3231         calculate D2E/DX2
analytically  !
 ! D62   D(4,18,26,27)          -4.8248         calculate D2E/DX2
analytically  !
 ! D63   D(19,18,26,24)          1.8233         calculate D2E/DX2
analytically  !
 ! D64   D(19,18,26,27)       -179.3246         calculate D2E/DX2
analytically  !
 ! D65   D(2,19,20,21)           3.3048         calculate D2E/DX2
analytically  !
 ! D66   D(2,19,20,22)        -177.0453         calculate D2E/DX2
analytically  !
 ! D67   D(18,19,20,21)        178.5189         calculate D2E/DX2
analytically  !
```

```
 ! D68   D(18,19,20,22)         -1.8312         calculate D2E/DX2
analytically  !
 ! D69   D(19,20,22,23)       -178.3902         calculate D2E/DX2
analytically  !
 ! D70   D(19,20,22,24)          1.9416         calculate D2E/DX2
analytically  !
 ! D71   D(21,20,22,23)          1.2533         calculate D2E/DX2
analytically  !
 ! D72   D(21,20,22,24)       -178.4149         calculate D2E/DX2
analytically  !
 ! D73   D(20,22,24,25)        179.7419         calculate D2E/DX2
analytically  !
 ! D74   D(20,22,24,26)         -0.1366         calculate D2E/DX2
analytically  !
 ! D75   D(23,22,24,25)          0.074          calculate D2E/DX2
analytically  !
 ! D76   D(23,22,24,26)       -179.8045         calculate D2E/DX2
analytically  !
 ! D77   D(22,24,26,18)         -1.7455         calculate D2E/DX2
analytically  !
 ! D78   D(22,24,26,27)        179.4159         calculate D2E/DX2
analytically  !
 ! D79   D(25,24,26,18)        178.3762         calculate D2E/DX2
analytically  !
 ! D80   D(25,24,26,27)         -0.4624         calculate D2E/DX2
analytically  !
 ! D81   D(8,28,30,29)          -8.0566         calculate D2E/DX2
analytically  !
 ! D82   D(32,28,30,29)        172.5401         calculate D2E/DX2
analytically  !
 ! D83   D(6,29,30,28)           8.3744         calculate D2E/DX2
analytically  !
 ! D84   D(31,29,30,28)       -172.3084         calculate D2E/DX2
analytically  !
 ---------------------------------------------------------------------
-----------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
 Number of steps in this run= 202 maximum allowed number of steps=
210.
 Search for a saddle point of order  1.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.579888    0.490113    1.140874
    2          6             0        0.563221    1.034727    0.424660
    3          6             0       -0.742362   -0.923222    1.092565
```

4	6	0	0.243221	-1.663023	0.349361
5	1	0	0.083270	-2.734020	0.232551
6	6	0	-0.200528	-0.938022	-1.652981
7	1	0	0.499349	-1.621354	-2.116646
8	6	0	-0.061131	0.467930	-1.629311
9	1	0	0.762893	1.020221	-2.061564
10	6	0	-1.572655	1.263020	1.789167
11	1	0	-1.485953	2.343063	1.834217
12	6	0	-2.658674	0.646513	2.389123
13	1	0	-3.401654	1.251265	2.901728
14	6	0	-2.816857	-0.752737	2.330409
15	1	0	-3.680539	-1.219981	2.795081
16	6	0	-1.878962	-1.528493	1.672488
17	1	0	-2.001031	-2.606284	1.603728
18	6	0	1.601570	-1.179385	0.353302
19	6	0	1.775957	0.230263	0.384237
20	6	0	3.081702	0.760316	0.279124
21	1	0	3.214138	1.836106	0.278175
22	6	0	4.173454	-0.090130	0.186300
23	1	0	5.175562	0.326783	0.132302
24	6	0	3.996047	-1.488350	0.154312
25	1	0	4.860270	-2.142639	0.077159
26	6	0	2.721289	-2.027508	0.218621
27	1	0	2.574225	-3.104627	0.185067
28	6	0	-1.429801	1.037590	-1.698214
29	6	0	-1.651016	-1.230402	-1.749085
30	8	0	-2.343229	-0.020136	-1.655503
31	8	0	-2.226757	-2.279584	-1.871352
32	8	0	-1.795831	2.181508	-1.767098
33	6	0	0.680314	2.531169	0.292087
34	1	0	-0.125972	3.139284	0.701758
35	8	0	1.622823	3.076958	-0.271771

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.454739	0.000000			
3	C	1.423463	2.446264	0.000000		
4	C	2.437211	2.717706	1.439108	0.000000	
5	H	3.414654	3.804039	2.168013	1.089157	0.000000
6	C	3.160555	2.965071	2.798540	2.175296	2.619424
7	H	4.029204	3.676558	3.511164	2.479623	2.632465
8	C	2.818426	2.220331	3.131771	2.923822	3.706732
9	H	3.512789	2.494271	3.998911	3.644505	4.451873
10	C	1.415364	2.544791	2.440142	3.732583	4.597985
11	H	2.176029	2.810286	3.430976	4.609074	5.550186
12	C	2.429802	3.793472	2.795958	4.232680	4.857681
13	H	3.412085	4.680063	3.882435	5.319094	5.928887
14	C	2.822003	4.272217	2.421746	3.757293	4.091116
15	H	3.908306	5.358368	3.408740	4.644752	4.798451
16	C	2.458653	3.753855	1.412276	2.504481	2.716076
17	H	3.438249	4.606794	2.162922	2.738584	2.498150

This journal is © The Royal Society of Chemistry 2014

18	C	2.857666	2.446539	2.471062	1.441885	2.176397
19	C	2.487977	1.455859	2.859053	2.436191	3.416895
20	C	3.771321	2.537564	4.256695	3.732892	4.604688
21	H	4.117108	2.773270	4.891934	4.590786	5.539898
22	C	4.882843	3.788918	5.067604	4.236427	4.870513
23	H	5.845434	4.675505	6.124250	5.323010	5.942222
24	C	5.082008	4.268876	4.863354	3.761949	4.107023
25	H	6.136627	5.355468	5.823016	4.649867	4.815974
26	C	4.252850	3.751932	3.738998	2.508139	2.731025
27	H	4.876900	4.608231	4.072079	2.745686	2.518821
28	C	3.013719	2.911827	3.479340	3.779534	4.499142
29	C	3.529780	3.841721	2.999164	2.859855	3.032408
30	O	3.345064	3.726562	3.306088	3.661732	4.100953
31	O	4.410998	4.903091	3.581613	3.378240	3.157395
32	O	3.577099	3.418192	4.350496	4.839168	5.629568
33	C	2.544496	1.506859	3.820679	4.217295	5.299266
34	H	2.723411	2.231800	4.127544	4.829352	5.895730
35	O	3.679575	2.403847	4.843238	4.975593	6.032581

		6	7	8	9	10
6	C	0.000000				
7	H	1.082477	0.000000			
8	C	1.413044	2.217373	0.000000		
9	H	2.220323	2.655260	1.082074	0.000000	
10	C	4.309954	5.279033	3.821369	4.510196	0.000000
11	H	4.957659	5.938632	4.188349	4.688745	1.084454
12	C	4.989172	5.951326	4.788208	5.626313	1.385448
13	H	5.982103	6.975231	5.683575	6.483140	2.140833
14	C	4.769371	5.614981	4.976287	5.936954	2.429868
15	H	5.654665	6.462014	5.960235	6.953387	3.408861
16	C	3.771544	4.474653	4.265219	5.236266	2.810691
17	H	4.078120	4.589463	4.864827	5.850229	3.897359
18	C	2.707579	2.740597	3.067405	3.372421	4.254733
19	C	3.069469	3.363425	2.736011	2.762657	3.775396
20	C	4.170182	4.252130	3.688497	3.305033	4.918941
21	H	4.804695	5.005924	4.029615	3.485491	5.052218
22	C	4.820124	4.598614	4.641076	4.232930	6.117023
23	H	5.804249	5.542560	5.526858	4.976500	7.011432
24	C	4.602218	4.171551	4.844485	4.653635	6.422868
25	H	5.482350	4.909394	5.826431	5.600564	7.477433
26	C	3.636879	3.248915	4.169403	4.280562	5.633129
27	H	3.971379	3.435563	4.795856	5.034148	6.232663
28	C	2.327273	3.311599	1.484088	2.222663	3.497578
29	C	1.482780	2.216306	2.329466	3.315102	4.329263
30	O	2.331027	3.294966	2.333852	3.300791	3.755799
31	O	2.439893	2.815154	3.506758	4.456781	5.135883
32	O	3.505636	4.455535	2.442236	2.825308	3.679735
33	C	4.073630	4.803977	2.915213	2.798117	2.987527
34	H	4.709010	5.567594	3.546015	3.593947	2.606860
35	O	4.620867	5.171063	3.389048	2.858847	4.212946

		11	12	13	14	15
11	H	0.000000				
12	C	2.135761	0.000000			

13	H	2.449799	1.086512	0.000000		
14	C	3.406096	1.409386	2.164351	0.000000	
15	H	4.293571	2.166289	2.489218	1.086363	0.000000
16	C	3.894812	2.419125	3.399511	1.383584	2.145012
17	H	4.981412	3.410283	4.304327	2.151575	2.482318
18	C	4.912591	5.062425	6.118397	4.859370	5.819331
19	C	4.148063	4.884545	5.847039	5.084075	6.139114
20	C	5.078078	6.116941	7.010919	6.425737	7.481946
21	H	4.976859	6.353043	7.140992	6.876531	7.950538
22	C	6.376907	7.216166	8.158134	7.341710	8.352695
23	H	7.165032	8.159088	9.060520	8.359175	9.376214
24	C	6.895950	7.337393	8.353428	7.189728	8.122540
25	H	7.967642	8.346201	9.367826	8.120791	9.010206
26	C	6.277972	6.387916	7.445794	6.062652	6.947924
27	H	6.991571	6.805303	7.878145	6.260802	7.034638
28	C	3.766362	4.285953	5.009324	4.621580	5.509278
29	C	5.063294	4.654347	5.554590	4.269616	4.976798
30	O	4.300904	4.111317	4.848204	4.080260	4.799555
31	O	5.970670	5.186544	6.052237	4.509354	5.001184
32	O	3.618231	4.513854	5.024137	5.142164	5.994642
33	C	2.665757	4.370164	5.011072	5.212389	6.273208
34	H	1.940613	3.933915	4.374309	5.004118	6.001678
35	O	3.826000	5.596306	6.216882	6.414722	7.482975

		16	17	18	19	20
16	C	0.000000				
17	H	1.086859	0.000000			
18	C	3.738480	4.071651	0.000000		
19	C	4.255731	4.878401	1.420731	0.000000	
20	C	5.638111	6.238810	2.441052	1.413144	0.000000
21	H	6.261334	6.977815	3.420410	2.158320	1.083912
22	C	6.396044	6.816480	2.798027	2.426896	1.387010
23	H	7.455235	7.891227	3.884688	3.410293	2.143305
24	C	6.068130	6.270210	2.422514	2.816966	2.430659
25	H	6.952661	7.044347	3.409287	3.903581	3.410461
26	C	4.850263	4.955180	1.411107	2.453286	2.811676
27	H	4.952524	4.816006	2.163543	3.434879	3.899252
28	C	4.260066	4.950449	4.279358	3.907079	4.933600
29	C	3.442089	3.641005	3.873235	4.292872	5.520436
30	O	3.683233	4.174667	4.576089	4.603361	5.812208
31	O	3.639217	3.497694	4.562413	5.235335	6.484233
32	O	5.059819	5.858970	5.228196	4.603615	5.476964
33	C	4.993622	5.941670	3.823699	2.550116	2.983748
34	H	5.079708	6.110724	4.664410	3.490065	4.015879
35	O	6.103509	6.996360	4.302049	2.925315	2.792605

		21	22	23	24	25
21	H	0.000000				
22	C	2.153860	0.000000			
23	H	2.479217	1.086716	0.000000		
24	C	3.417416	1.409793	2.164821	0.000000	
25	H	4.310519	2.167123	2.490079	1.086705	0.000000
26	C	3.895377	2.421417	3.401998	1.385581	2.146743
27	H	4.982871	3.412437	4.306311	2.152876	2.482552

This journal is © The Royal Society of Chemistry 2014

28	C	5.109786	6.018273	6.891071	6.265146	7.268480
29	C	6.097785	6.242627	7.250283	5.964795	6.823796
30	O	6.170014	6.772318	7.736202	6.754073	7.706980
31	O	7.152811	7.070385	8.099513	6.591863	7.351286
32	O	5.422383	6.678957	7.459762	7.120781	8.148817
33	C	2.627465	4.368573	5.009202	5.212447	6.273971
34	H	3.610267	5.401840	6.028325	6.221393	7.290504
35	O	2.091516	4.092187	4.510952	5.162923	6.151992

		26	27	28	29	30
26	C	0.000000				
27	H	1.087630	0.000000			
28	C	5.504601	6.061100	0.000000		
29	C	4.860483	5.010621	2.279323	0.000000	
30	O	5.761183	6.089592	1.398199	1.397376	0.000000
31	O	5.377238	5.287625	3.415957	1.203000	2.272721
32	O	6.485620	7.131028	1.203026	3.415029	2.271417
33	C	4.995249	5.946474	3.262616	4.873489	4.409544
34	H	5.919126	6.822350	3.446296	5.237036	4.522703
35	O	5.244300	6.271033	3.938563	5.608371	5.218838

		31	32	33	34	35
31	O	0.000000				
32	O	4.483069	0.000000			
33	C	6.022863	3.239413	0.000000		
34	H	6.355968	3.130657	1.089831	0.000000	
35	O	6.787523	3.837321	1.226436	2.002480	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.579888	0.490113	1.140874
2	6	0	0.563221	1.034727	0.424660
3	6	0	-0.742362	-0.923222	1.092565
4	6	0	0.243221	-1.663023	0.349361
5	1	0	0.083270	-2.734020	0.232551
6	6	0	-0.200528	-0.938022	-1.652981
7	1	0	0.499349	-1.621354	-2.116646
8	6	0	-0.061131	0.467930	-1.629311
9	1	0	0.762893	1.020221	-2.061564
10	6	0	-1.572655	1.263020	1.789167
11	1	0	-1.485953	2.343063	1.834217
12	6	0	-2.658674	0.646513	2.389123
13	1	0	-3.401654	1.251265	2.901728
14	6	0	-2.816857	-0.752737	2.330409
15	1	0	-3.680539	-1.219981	2.795081
16	6	0	-1.878962	-1.528493	1.672488

```
   17          1             0       -2.001031   -2.606284    1.603728
   18          6             0        1.601570   -1.179385    0.353302
   19          6             0        1.775957    0.230263    0.384237
   20          6             0        3.081702    0.760316    0.279124
   21          1             0        3.214138    1.836106    0.278175
   22          6             0        4.173454   -0.090130    0.186300
   23          1             0        5.175562    0.326783    0.132302
   24          6             0        3.996047   -1.488350    0.154312
   25          1             0        4.860270   -2.142639    0.077159
   26          6             0        2.721289   -2.027508    0.218621
   27          1             0        2.574225   -3.104627    0.185067
   28          6             0       -1.429801    1.037590   -1.698214
   29          6             0       -1.651016   -1.230402   -1.749085
   30          8             0       -2.343229   -0.020136   -1.655503
   31          8             0       -2.226757   -2.279584   -1.871352
   32          8             0       -1.795831    2.181508   -1.767098
   33          6             0        0.680314    2.531169    0.292087
   34          1             0       -0.125972    3.139284    0.701758
   35          8             0        1.622823    3.076958   -0.271771
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3985487      0.2621116
0.2442286
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1915.6196091740 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1032.13507368     A.U. after   17 cycles
             Convg  =    0.7618D-08             -V/T =  2.0093
             S**2   =   0.0000
 Range of M.O.s used for correlation:     1   456
 NBasis=   461 NAE=    79 NBE=    79 NFC=     0 NFV=     0
 NROrb=    456 NOA=    79 NOB=    79 NVA=   377 NVB=   377

 **** Warning!!: The largest alpha MO coefficient is  0.18783387D+03

 Symmetrizing basis deriv contribution to polar:
 IMax=3 JMax=2 DiffMx= 0.00D+00
 G2DrvN: will do   36 centers at a time, making    1 passes doing
MaxLOS=2.
 FoFDir/FoFCou used for L=0 through L=2.
 DoAtom=TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT
          Differentiating once with respect to electric field.
                with respect to dipole field.
```

```
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 2 Meth= 1.
 IRaf=       0 NMat= 108 IRICut=     108 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
          There are 108 degrees of freedom in the 1st order CPHF.
   105 vectors were produced by pass  0.
 AX will form 105 AO Fock derivatives at one time.
   105 vectors were produced by pass  1.
   105 vectors were produced by pass  2.
   105 vectors were produced by pass  3.
    99 vectors were produced by pass  4.
    16 vectors were produced by pass  5.
     3 vectors were produced by pass  6.
     3 vectors were produced by pass  7.
     3 vectors were produced by pass  8.
 Inv2:  IOpt= 1 Iter= 1 AM= 3.32D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension  544 with in-core refinement.
 Isotropic polarizability for W=    0.000000      239.43 Bohr**3.
 End of Minotr Frequency-dependent properties file   721 does not
exist.

**********************************************************************

            Population analysis using the SCF density.

**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.22673 -19.17777 -19.17321 -19.17308 -
10.34623
 Alpha  occ. eigenvalues --  -10.34601 -10.30354 -10.25987 -10.25676 -
10.24711
 Alpha  occ. eigenvalues --  -10.24560 -10.23837 -10.23472 -10.23380 -
10.23338
 Alpha  occ. eigenvalues --  -10.22276 -10.22263 -10.22176 -10.22119 -
10.22096
 Alpha  occ. eigenvalues --  -10.21964 -10.21846 -10.21366  -1.14571
-1.08175
 Alpha  occ. eigenvalues --   -1.06847  -1.04324  -0.92343  -0.88251
-0.84747
 Alpha  occ. eigenvalues --   -0.82644  -0.82165  -0.77976  -0.77294
-0.74291
 Alpha  occ. eigenvalues --   -0.70585  -0.69071  -0.66503  -0.64264
-0.63661
 Alpha  occ. eigenvalues --   -0.62501  -0.60067  -0.58881  -0.57050
-0.55224
 Alpha  occ. eigenvalues --   -0.53360  -0.51544  -0.50547  -0.50000
-0.49386
 Alpha  occ. eigenvalues --   -0.49024  -0.48027  -0.47623  -0.46942
-0.46053
 Alpha  occ. eigenvalues --   -0.45058  -0.44848  -0.44459  -0.44092
-0.43770
 Alpha  occ. eigenvalues --   -0.42577  -0.42211  -0.41048  -0.40583
-0.40162
 Alpha  occ. eigenvalues --   -0.38845  -0.37587  -0.37159  -0.36715
-0.35560
 Alpha  occ. eigenvalues --   -0.33795  -0.32851  -0.32017  -0.29506
-0.28379
 Alpha  occ. eigenvalues --   -0.27820  -0.27569  -0.27161  -0.24718
 Alpha virt. eigenvalues --   -0.11487  -0.09003  -0.05561  -0.04104
-0.03201
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --   -0.00895  -0.00731  -0.00194   0.00310
0.00775
 Alpha virt. eigenvalues --    0.01108   0.01940   0.02248   0.03190
0.03379
 Alpha virt. eigenvalues --    0.03793   0.03976   0.04404   0.04752
0.06014
 Alpha virt. eigenvalues --    0.06152   0.06334   0.06537   0.06853
0.07453
 Alpha virt. eigenvalues --    0.08088   0.08390   0.08822   0.09852
0.10022
 Alpha virt. eigenvalues --    0.10103   0.10458   0.11153   0.11346
0.11619
 Alpha virt. eigenvalues --    0.12316   0.12463   0.12990   0.13274
0.13511
 Alpha virt. eigenvalues --    0.13782   0.14178   0.14413   0.14523
0.15208
 Alpha virt. eigenvalues --    0.15532   0.15950   0.16108   0.16306
0.16656
 Alpha virt. eigenvalues --    0.16899   0.17286   0.17651   0.18114
0.18265
 Alpha virt. eigenvalues --    0.18586   0.18860   0.19144   0.19437
0.19490
 Alpha virt. eigenvalues --    0.20106   0.20328   0.20746   0.20879
0.21389
 Alpha virt. eigenvalues --    0.21788   0.22082   0.22371   0.22783
0.22946
 Alpha virt. eigenvalues --    0.23044   0.23317   0.23563   0.24159
0.24492
 Alpha virt. eigenvalues --    0.24521   0.25075   0.25395   0.25578
0.26203
 Alpha virt. eigenvalues --    0.26388   0.26630   0.27058   0.27385
0.27743
 Alpha virt. eigenvalues --    0.27920   0.28348   0.28683   0.28780
0.28879
 Alpha virt. eigenvalues --    0.29254   0.29594   0.29831   0.29990
0.30795
 Alpha virt. eigenvalues --    0.31150   0.31833   0.31914   0.32826
0.33408
 Alpha virt. eigenvalues --    0.33802   0.34180   0.34737   0.34920
0.35267
 Alpha virt. eigenvalues --    0.35630   0.35944   0.36379   0.36588
0.37052
 Alpha virt. eigenvalues --    0.37148   0.38008   0.38581   0.39174
0.40304
 Alpha virt. eigenvalues --    0.40425   0.41703   0.41862   0.42187
0.42992
 Alpha virt. eigenvalues --    0.43477   0.43972   0.44484   0.45575
0.46024
 Alpha virt. eigenvalues --    0.47836   0.49726   0.51573   0.51763
0.54047
 Alpha virt. eigenvalues --    0.56257   0.57407   0.58000   0.59923
0.62426
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.63971   0.65879   0.67206   0.68824
0.69173
 Alpha virt. eigenvalues --    0.69705   0.70229   0.71132   0.72003
0.72480
 Alpha virt. eigenvalues --    0.72827   0.73204   0.73688   0.74512
0.75058
 Alpha virt. eigenvalues --    0.75461   0.75818   0.76135   0.76785
0.77921
 Alpha virt. eigenvalues --    0.78652   0.79556   0.80804   0.81077
0.81532
 Alpha virt. eigenvalues --    0.82621   0.83133   0.83768   0.84614
0.85621
 Alpha virt. eigenvalues --    0.87010   0.87274   0.88340   0.88911
0.89871
 Alpha virt. eigenvalues --    0.90823   0.91402   0.92295   0.92705
0.93279
 Alpha virt. eigenvalues --    0.93954   0.94260   0.95374   0.95867
0.96978
 Alpha virt. eigenvalues --    0.97572   0.99522   1.00850   1.00925
1.02661
 Alpha virt. eigenvalues --    1.03443   1.04324   1.05531   1.06583
1.07440
 Alpha virt. eigenvalues --    1.07570   1.09877   1.10587   1.11834
1.13449
 Alpha virt. eigenvalues --    1.13956   1.14962   1.15579   1.16998
1.17624
 Alpha virt. eigenvalues --    1.19443   1.19947   1.20749   1.21384
1.22422
 Alpha virt. eigenvalues --    1.24787   1.25324   1.25787   1.26704
1.27607
 Alpha virt. eigenvalues --    1.28344   1.28864   1.29187   1.30590
1.31294
 Alpha virt. eigenvalues --    1.32424   1.34294   1.35083   1.35819
1.36986
 Alpha virt. eigenvalues --    1.37775   1.38755   1.39145   1.39919
1.40304
 Alpha virt. eigenvalues --    1.41011   1.41934   1.42790   1.43389
1.43949
 Alpha virt. eigenvalues --    1.45024   1.45450   1.45703   1.46582
1.46959
 Alpha virt. eigenvalues --    1.48298   1.48755   1.49316   1.50750
1.51514
 Alpha virt. eigenvalues --    1.52408   1.53371   1.55080   1.56836
1.58423
 Alpha virt. eigenvalues --    1.59587   1.64301   1.66272   1.67520
1.68859
 Alpha virt. eigenvalues --    1.73052   1.74550   1.75460   1.76411
1.78641
 Alpha virt. eigenvalues --    1.79339   1.80415   1.81438   1.82821
1.83360
 Alpha virt. eigenvalues --    1.83641   1.84036   1.85668   1.86706
1.87609
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    1.88225   1.89057   1.89995   1.90111
1.92669
 Alpha virt. eigenvalues --    1.92966   1.94201   1.94895   1.96038
1.96559
 Alpha virt. eigenvalues --    1.97848   1.98081   1.98992   1.99578
2.02965
 Alpha virt. eigenvalues --    2.03407   2.04574   2.06345   2.07043
2.08606
 Alpha virt. eigenvalues --    2.09200   2.10411   2.11618   2.12251
2.13789
 Alpha virt. eigenvalues --    2.15332   2.16690   2.18610   2.18836
2.19718
 Alpha virt. eigenvalues --    2.20478   2.23657   2.25073   2.25753
2.26433
 Alpha virt. eigenvalues --    2.27626   2.28178   2.29232   2.30775
2.31484
 Alpha virt. eigenvalues --    2.32607   2.33192   2.34348   2.36685
2.39068
 Alpha virt. eigenvalues --    2.41257   2.43062   2.45207   2.47295
2.48957
 Alpha virt. eigenvalues --    2.49835   2.55163   2.56886   2.58436
2.59107
 Alpha virt. eigenvalues --    2.61496   2.62034   2.63244   2.65265
2.66097
 Alpha virt. eigenvalues --    2.68610   2.69727   2.71600   2.71974
2.74281
 Alpha virt. eigenvalues --    2.75223   2.75633   2.79757   2.80697
2.82864
 Alpha virt. eigenvalues --    2.84866   2.85674   2.87403   2.89666
2.90143
 Alpha virt. eigenvalues --    2.93538   2.94006   2.96860   2.99168
3.10728
 Alpha virt. eigenvalues --    3.11134   3.17836   3.18315   3.21988
3.24052
 Alpha virt. eigenvalues --    3.24844   3.34432   3.41273   3.42732
4.24746
 Alpha virt. eigenvalues --    4.28735   4.30744   4.32341   4.33205
4.35199
 Alpha virt. eigenvalues --    4.36557   4.38038   4.40609   4.44925
4.47467
 Alpha virt. eigenvalues --    4.49353   4.50607   4.50763   4.54451
4.57972
 Alpha virt. eigenvalues --    4.63827   4.68304   4.69924   4.75460
4.84265
 Alpha virt. eigenvalues --    4.95239   5.30652
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   41.411912 -13.456465  16.732648 -13.659147   0.027042
0.609730
     2  C  -13.456465  35.016561 -14.195025  13.971781  -0.028854  -
1.753553
```

This journal is © The Royal Society of Chemistry 2014

```
     3  C   16.732648 -14.195025  36.488923 -19.401056   0.031145
1.162654
     4  C  -13.659147  13.971781 -19.401056  35.746357   0.183430  -
1.741787
     5  H    0.027042  -0.028854   0.031145   0.183430   0.521647
0.006998
     6  C    0.609730  -1.753553   1.162654  -1.741787   0.006998
9.835645
     7  H    0.017961  -0.022630   0.028541  -0.067089  -0.001434
0.382064
     8  C   -1.050703   0.432859  -1.036418   0.428979   0.013324  -
2.803957
     9  H   -0.026835  -0.013225   0.005734   0.008745  -0.000040  -
0.021931
    10  C  -15.761889   4.601612  -7.929065   3.718583  -0.007589  -
0.198100
    11  H   -0.041670  -0.032940   0.059013   0.021212   0.000002
0.000360
    12  C   -1.600628   0.047790   0.171398   0.905567   0.003153  -
0.208520
    13  H   -0.009914  -0.014017   0.024370   0.002522   0.000000
0.001824
    14  C    0.245941   0.338105  -2.017977  -0.406131   0.012919
0.120440
    15  H    0.024843   0.000935   0.007060  -0.016331  -0.000007  -
0.001611
    16  C   -8.585302   3.597506 -13.233961   7.123519   0.008802  -
0.171585
    17  H    0.079199   0.019930  -0.061902  -0.030564   0.004010  -
0.012499
    18  C    2.484804  -7.511873   6.131217  -9.983466   0.008581
0.691747
    19  C   -0.358421 -14.379414   4.698286 -14.757505   0.028288
1.845671
    20  C    1.431947   2.811004  -0.157728   1.376808   0.010870  -
0.295657
    21  H    0.001385  -0.020488  -0.000268   0.005334   0.000002  -
0.001862
    22  C    0.182988  -1.830225   0.229428  -0.754055   0.001297  -
0.000553
    23  H   -0.003399  -0.010926  -0.000081   0.003258   0.000000  -
0.000072
    24  C   -0.450334   0.667828  -0.778251   0.923773  -0.012712
0.021021
    25  H   -0.000045   0.003414  -0.003452  -0.003315  -0.000007  -
0.000465
    26  C   -0.462660  -1.899045   1.047579  -0.642889  -0.007282
0.108288
    27  H    0.000102   0.004461  -0.008406  -0.030571   0.003693
0.002460
    28  C   -0.046971   0.631945   0.041740   0.218612   0.001335
1.236320
```

This journal is © The Royal Society of Chemistry 2014

29	C	-0.424583	0.827003	-0.819829	1.509195	-0.030975	-1.814176
30	O	-0.081625	0.103846	-0.188831	0.136514	0.000061	-0.406140
31	O	0.042893	-0.063878	0.242976	-0.188412	0.004950	-0.053576
32	O	0.161366	-0.126759	0.060526	-0.055171	0.000031	-0.056107
33	C	-1.825874	-1.217611	-1.186156	0.970318	0.003260	-0.326181
34	H	0.091392	-0.239552	0.001623	0.017498	0.000000	0.004979
35	O	0.012084	0.188614	-0.050665	0.043527	-0.000013	0.018974

		7	8	9	10	11	12
1	C	0.017961	-1.050703	-0.026835	-15.761889	-0.041670	-1.600628
2	C	-0.022630	0.432859	-0.013225	4.601612	-0.032940	0.047790
3	C	0.028541	-1.036418	0.005734	-7.929065	0.059013	0.171398
4	C	-0.067089	0.428979	0.008745	3.718583	0.021212	0.905567
5	H	-0.001434	0.013324	-0.000040	-0.007589	0.000002	0.003153
6	C	0.382064	-2.803957	-0.021931	-0.198100	0.000360	-0.208520
7	H	0.464293	-0.028305	-0.002040	-0.002999	0.000000	0.000037
8	C	-0.028305	10.774927	0.380401	1.121117	-0.005801	0.365167
9	H	-0.002040	0.380401	0.445168	0.023001	-0.000001	0.001730
10	C	-0.002999	1.121117	0.023001	20.166939	0.247028	-1.382324
11	H	0.000000	-0.005801	-0.000001	0.247028	0.548397	0.099980
12	C	0.000037	0.365167	0.001730	-1.382324	0.099980	9.406178
13	H	0.000000	-0.002635	0.000000	0.047659	-0.004793	0.257768
14	C	0.000673	0.005258	0.000744	-0.336957	-0.005846	0.776984
15	H	0.000000	0.000878	0.000000	0.020583	-0.000170	-0.041403
16	C	0.007337	0.537115	-0.002049	7.066022	-0.025354	-1.010273
17	H	0.000001	0.006600	0.000000	-0.027154	0.000017	0.005845
18	C	0.058912	-0.989382	-0.005731	-2.251131	-0.008030	-0.748878

This journal is © The Royal Society of Chemistry 2014

19	C	0.024256	-0.873936	0.065071	-0.943002	-0.050716	-1.002373
20	C	-0.004981	-0.322616	-0.054063	-2.025087	0.001949	0.033534
21	H	0.000001	-0.000554	-0.000110	-0.002623	-0.000002	-0.000276
22	C	0.004957	0.059821	-0.010000	0.066306	-0.000885	0.008453
23	H	0.000000	0.000199	0.000001	0.000344	0.000000	0.000020
24	C	-0.014780	-0.126929	-0.002925	-0.058979	0.000068	-0.004843
25	H	0.000002	0.000236	0.000000	-0.000104	0.000000	0.000007
26	C	-0.030172	-0.397223	-0.001098	-0.909751	-0.000172	-0.106279
27	H	-0.000033	-0.000275	0.000000	0.000132	0.000000	-0.000135
28	C	0.013797	-2.575374	-0.088105	-0.442172	0.013978	-0.255098
29	C	-0.084076	1.166295	0.018001	0.094275	-0.002138	0.150714
30	O	0.007724	-0.178258	0.007854	-0.010279	-0.000037	0.036148
31	O	0.001666	-0.074853	-0.000561	-0.021085	0.000001	-0.009394
32	O	-0.000654	-0.052417	0.003596	-0.080751	0.000308	-0.021133
33	C	-0.005775	1.113822	-0.013384	1.608166	-0.002053	0.445849
34	H	0.000001	-0.002730	0.000193	0.005113	0.007873	0.045822
35	O	-0.000052	-0.030144	0.005354	0.067324	0.002207	0.034793

		13	14	15	16	17	18
1	C	-0.009914	0.245941	0.024843	-8.585302	0.079199	2.484804
2	C	-0.014017	0.338105	0.000935	3.597506	0.019930	-7.511873
3	C	0.024370	-2.017977	0.007060	-13.233961	-0.061902	6.131217
4	C	0.002522	-0.406131	-0.016331	7.123519	-0.030564	-9.983466
5	H	0.000000	0.012919	-0.000007	0.008802	0.004010	0.008581
6	C	0.001824	0.120440	-0.001611	-0.171585	-0.012499	0.691747
7	H	0.000000	0.000673	0.000000	0.007337	0.000001	0.058912
8	C	-0.002635	0.005258	0.000878	0.537115	0.006600	-0.989382

This journal is © The Royal Society of Chemistry 2014

9	H	0.000000	0.000744	0.000000	-0.002049	0.000000	-0.005731
10	C	0.047659	-0.336957	0.020583	7.066022	-0.027154	-2.251131
11	H	-0.004793	-0.005846	-0.000170	-0.025354	0.000017	-0.008030
12	C	0.257768	0.776984	-0.041403	-1.010273	0.005845	-0.748878
13	H	0.520327	-0.029215	-0.004140	0.019217	-0.000161	0.002091
14	C	-0.029215	6.942097	0.293768	0.991210	0.074565	-0.365951
15	H	-0.004140	0.293768	0.519131	0.007029	-0.004321	-0.002086
16	C	0.019217	0.991210	0.007029	15.899874	0.262484	-2.394470
17	H	-0.000161	0.074565	-0.004321	0.262484	0.527830	-0.041970
18	C	0.002091	-0.365951	-0.002086	-2.394470	-0.041970	18.708874
19	C	-0.001256	-0.026270	0.001520	-2.528084	-0.005590	9.162329
20	C	0.000138	-0.065553	-0.000231	-0.807673	0.000439	-2.066063
21	H	0.000000	-0.000100	0.000000	0.000551	0.000000	0.054439
22	C	0.000021	0.010133	0.000012	-0.026627	-0.000129	1.218338
23	H	0.000000	0.000002	0.000000	-0.000115	0.000000	0.006611
24	C	0.000009	-0.021147	-0.000005	-0.039741	-0.000188	-1.741626
25	H	0.000000	0.000002	0.000000	0.000144	0.000000	-0.000763
26	C	-0.000125	-0.138439	0.000153	-1.186158	0.001247	-1.868044
27	H	0.000000	0.000488	0.000000	0.003177	0.000002	-0.035342
28	C	0.003538	-0.001675	-0.001463	-0.088784	-0.003229	0.340818
29	C	-0.002007	-0.104770	0.002940	0.130463	0.009669	-0.534327
30	O	-0.000024	0.013925	-0.000022	-0.006581	0.000257	-0.035231
31	O	0.000002	-0.021458	-0.000087	-0.124670	0.000102	0.060433
32	O	-0.000113	0.001706	0.000001	-0.014183	0.000000	0.009059
33	C	-0.002948	0.090333	0.000270	0.559967	0.000920	-2.103916
34	H	-0.000001	0.000042	0.000000	-0.003437	0.000000	-0.032073

This journal is © The Royal Society of Chemistry 2014

35	O	-0.000001	0.001854	0.000000	-0.009742	-0.000001	-0.077475

		19	20	21	22	23	24
1	C	-0.358421	1.431947	0.001385	0.182988	-0.003399	-0.450334
2	C	-14.379414	2.811004	-0.020488	-1.830225	-0.010926	0.667828
3	C	4.698286	-0.157728	-0.000268	0.229428	-0.000081	-0.778251
4	C	-14.757505	1.376808	0.005334	-0.754055	0.003258	0.923773
5	H	0.028288	0.010870	0.000002	0.001297	0.000000	-0.012712
6	C	1.845671	-0.295657	-0.001862	-0.000553	-0.000072	0.021021
7	H	0.024256	-0.004981	0.000001	0.004957	0.000000	-0.014780
8	C	-0.873936	-0.322616	-0.000554	0.059821	0.000199	-0.126929
9	H	0.065071	-0.054063	-0.000110	-0.010000	0.000001	-0.002925
10	C	-0.943002	-2.025087	-0.002623	0.066306	0.000344	-0.058979
11	H	-0.050716	0.001949	-0.000002	-0.000885	0.000000	0.000068
12	C	-1.002373	0.033534	-0.000276	0.008453	0.000020	-0.004843
13	H	-0.001256	0.000138	0.000000	0.000021	0.000000	0.000009
14	C	-0.026270	-0.065553	-0.000100	0.010133	0.000002	-0.021147
15	H	0.001520	-0.000231	0.000000	0.000012	0.000000	-0.000005
16	C	-2.528084	-0.807673	0.000551	-0.026627	-0.000115	-0.039741
17	H	-0.005590	0.000439	0.000000	-0.000129	0.000000	-0.000188
18	C	9.162329	-2.066063	0.054439	1.218338	0.006611	-1.741626
19	C	46.000190	-15.607947	-0.191524	2.698235	0.015861	-1.095278
20	C	-15.607947	20.600190	0.324745	-3.428609	0.017811	0.472024
21	H	-0.191524	0.324745	0.486774	0.145779	-0.004216	0.019760
22	C	2.698235	-3.428609	0.145779	8.357543	0.299593	0.375644
23	H	0.015861	0.017811	-0.004216	0.299593	0.520232	-0.039328
24	C	-1.095278	0.472024	0.019760	0.375644	-0.039328	7.253335

This journal is © The Royal Society of Chemistry 2014

25	H	0.017673	0.022461	-0.000150	-0.042565	-0.003991
0.297515						
26	C	-2.733091	3.843304	-0.016826	-1.032612	0.008271
0.466935						
27	H	0.064190	-0.029166	0.000016	0.006602	-0.000159
0.029848						
28	C	0.323559	0.174566	0.001827	0.033301	0.000078
0.001344						
29	C	-0.959508	0.029144	-0.000525	-0.048719	-0.000061
0.122632						
30	O	-0.028234	0.019164	0.000001	-0.002671	0.000000
0.002822						
31	O	0.038950	0.003658	0.000000	0.000701	0.000000
-0.001989						
32	O	0.002065	0.008037	-0.000017	-0.001653	0.000000
0.000123						
33	C	-3.220658	-0.096971	-0.021085	-0.079937	-0.001044
-0.072024						
34	H	-0.116548	0.003851	-0.000167	0.000213	0.000000
-0.000216						
35	O	-0.394172	0.004586	-0.012519	0.039731	0.000248
-0.003246						

		25	26	27	28	29	30
1	C	-0.000045	-0.462660	0.000102	-0.046971	-0.424583	
-0.081625							
2	C	0.003414	-1.899045	0.004461	0.631945	0.827003	
0.103846							
3	C	-0.003452	1.047579	-0.008406	0.041740	-0.819829	
-0.188831							
4	C	-0.003315	-0.642889	-0.030571	0.218612	1.509195	
0.136514							
5	H	-0.000007	-0.007282	0.003693	0.001335	-0.030975	
0.000061							
6	C	-0.000465	0.108288	0.002460	1.236320	-1.814176	
-0.406140							
7	H	0.000002	-0.030172	-0.000033	0.013797	-0.084076	
0.007724							
8	C	0.000236	-0.397223	-0.000275	-2.575374	1.166295	
-0.178258							
9	H	0.000000	-0.001098	0.000000	-0.088105	0.018001	
0.007854							
10	C	-0.000104	-0.909751	0.000132	-0.442172	0.094275	
-0.010279							
11	H	0.000000	-0.000172	0.000000	0.013978	-0.002138	
-0.000037							
12	C	0.000007	-0.106279	-0.000135	-0.255098	0.150714	
0.036148							
13	H	0.000000	-0.000125	0.000000	0.003538	-0.002007	
-0.000024							
14	C	0.000002	-0.138439	0.000488	-0.001675	-0.104770	
0.013925							

This journal is © The Royal Society of Chemistry 2014

15	H	0.000000	0.000153	0.000000	-0.001463	0.002940	-0.000022
16	C	0.000144	-1.186158	0.003177	-0.088784	0.130463	-0.006581
17	H	0.000000	0.001247	0.000002	-0.003229	0.009669	0.000257
18	C	-0.000763	-1.868044	-0.035342	0.340818	-0.534327	-0.035231
19	C	0.017673	-2.733091	0.064190	0.323559	-0.959508	-0.028234
20	C	0.022461	3.843304	-0.029166	0.174566	0.029144	0.019164
21	H	-0.000150	-0.016826	0.000016	0.001827	-0.000525	0.000001
22	C	-0.042565	-1.032612	0.006602	0.033301	-0.048719	-0.002671
23	H	-0.003991	0.008271	-0.000159	0.000078	-0.000061	0.000000
24	C	0.297515	0.466935	0.029848	0.001344	0.122632	0.002822
25	H	0.522101	0.005188	-0.004339	-0.000055	0.000086	0.000000
26	C	0.005188	11.707991	0.271354	0.102250	-0.074625	0.023699
27	H	-0.004339	0.271354	0.533472	-0.000864	0.002305	0.000004
28	C	-0.000055	0.102250	-0.000864	7.450132	-1.162926	0.255220
29	C	0.000086	-0.074625	0.002305	-1.162926	6.827026	0.320649
30	O	0.000000	0.023699	0.000004	0.255220	0.320649	8.314452
31	O	0.000000	0.017682	0.000007	0.039049	0.433452	-0.083679
32	O	0.000000	0.000589	0.000000	0.414575	0.036403	-0.073230
33	C	0.000728	-0.236605	0.000754	-0.669923	0.153466	0.041135
34	H	0.000000	-0.002750	0.000000	0.012454	-0.000426	-0.000258
35	O	0.000014	-0.019015	-0.000005	-0.006205	-0.002824	-0.000011

		31	32	33	34	35
1	C	0.042893	0.161366	-1.825874	0.091392	0.012084
2	C	-0.063878	-0.126759	-1.217611	-0.239552	0.188614
3	C	0.242976	0.060526	-1.186156	0.001623	-0.050665
4	C	-0.188412	-0.055171	0.970318	0.017498	0.043527
5	H	0.004950	0.000031	0.003260	0.000000	-0.000013
6	C	-0.053576	-0.056107	-0.326181	0.004979	0.018974
7	H	0.001666	-0.000654	-0.005775	0.000001	-0.000052
8	C	-0.074853	-0.052417	1.113822	-0.002730	-0.030144
9	H	-0.000561	0.003596	-0.013384	0.000193	0.005354

This journal is © The Royal Society of Chemistry 2014

10	C	-0.021085	-0.080751	1.608166	0.005113	0.067324
11	H	0.000001	0.000308	-0.002053	0.007873	0.002207
12	C	-0.009394	-0.021133	0.445849	0.045822	0.034793
13	H	0.000002	-0.000113	-0.002948	-0.000001	-0.000001
14	C	-0.021458	0.001706	0.090333	0.000042	0.001854
15	H	-0.000087	0.000001	0.000270	0.000000	0.000000
16	C	-0.124670	-0.014183	0.559967	-0.003437	-0.009742
17	H	0.000102	0.000000	0.000920	0.000000	-0.000001
18	C	0.060433	0.009059	-2.103916	-0.032073	-0.077475
19	C	0.038950	0.002065	-3.220658	-0.116548	-0.394172
20	C	0.003658	0.008037	-0.096971	0.003851	0.004586
21	H	0.000000	-0.000017	-0.021085	-0.000167	-0.012519
22	C	0.000701	-0.001653	-0.079937	0.000213	0.039731
23	H	0.000000	0.000000	-0.001044	0.000000	0.000248
24	C	-0.001989	0.000123	-0.072024	-0.000216	-0.003246
25	H	0.000000	0.000000	0.000728	0.000000	0.000014
26	C	0.017682	0.000589	-0.236605	-0.002750	-0.019015
27	H	0.000007	0.000000	0.000754	0.000000	-0.000005
28	C	0.039049	0.414575	-0.669923	0.012454	-0.006205
29	C	0.433452	0.036403	0.153466	-0.000426	-0.002824
30	O	-0.083679	-0.073230	0.041135	-0.000258	-0.000011
31	O	8.145629	0.000072	-0.001123	-0.000001	-0.000005
32	O	0.000072	8.085743	0.036135	-0.000069	0.001417
33	C	-0.001123	0.036135	10.954638	0.460391	0.518989
34	H	-0.000001	-0.000069	0.460391	0.606344	-0.033355
35	O	-0.000005	0.001417	0.518989	-0.033355	7.983713

Mulliken atomic charges:

		1
1	C	0.288233
2	C	-0.448712
3	C	-0.095791
4	C	0.421959
5	H	0.214075
6	C	-0.180841
7	H	0.252800
8	C	0.145513
9	H	0.276504
10	C	-0.463162
11	H	0.178217
12	C	-0.405383
13	H	0.191869
14	C	-0.379697
15	H	0.192756
16	C	0.044373
17	H	0.194590
18	C	-0.140424
19	C	0.287385
20	C	-0.227886
21	H	0.232700
22	C	-0.479856
23	H	0.190865
24	C	-0.190140

This journal is © The Royal Society of Chemistry 2014

```
   25  H    0.189679
   26  C    0.160333
   27  H    0.186227
   28  C    0.032404
   29  C    0.232776
   30  O   -0.188362
   31  O   -0.387454
   32  O   -0.339495
   33  C    0.124128
   34  H    0.173797
   35  O   -0.283979
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  C    0.288233
    2  C   -0.448712
    3  C   -0.095791
    4  C    0.636034
    5  H    0.000000
    6  C    0.071959
    7  H    0.000000
    8  C    0.422017
    9  H    0.000000
   10  C   -0.284945
   11  H    0.000000
   12  C   -0.213514
   13  H    0.000000
   14  C   -0.186941
   15  H    0.000000
   16  C    0.238963
   17  H    0.000000
   18  C   -0.140424
   19  C    0.287385
   20  C    0.004815
   21  H    0.000000
   22  C   -0.288991
   23  H    0.000000
   24  C   -0.000461
   25  H    0.000000
   26  C    0.346560
   27  H    0.000000
   28  C    0.032404
   29  C    0.232776
   30  O   -0.188362
   31  O   -0.387454
   32  O   -0.339495
   33  C    0.297926
   34  H    0.000000
   35  O   -0.283979
Sum of Mulliken charges=   0.00000
APT atomic charges:
             1
```

This journal is © The Royal Society of Chemistry 2014

1	C	-0.052057
2	C	0.043409
3	C	-0.118718
4	C	0.367166
5	H	0.010866
6	C	-0.288993
7	H	0.041314
8	C	-0.200569
9	H	0.049129
10	C	-0.029641
11	H	0.044824
12	C	-0.001308
13	H	0.032869
14	C	-0.029640
15	H	0.034181
16	C	0.016759
17	H	0.039321
18	C	-0.106570
19	C	-0.062827
20	C	-0.045261
21	H	0.093129
22	C	-0.013892
23	H	0.028400
24	C	-0.028888
25	H	0.029314
26	C	-0.011058
27	H	0.031107
28	C	1.074113
29	C	1.110599
30	O	-0.744130
31	O	-0.728467
32	O	-0.686764
33	C	0.749158
34	H	-0.006063
35	O	-0.640813

Sum of APT charges= 0.00000

APT Atomic charges with hydrogens summed into heavy atoms:

		1
1	C	-0.052057
2	C	0.043409
3	C	-0.118718
4	C	0.378032
5	H	0.000000
6	C	-0.247680
7	H	0.000000
8	C	-0.151439
9	H	0.000000
10	C	0.015183
11	H	0.000000
12	C	0.031561
13	H	0.000000
14	C	0.004541

This journal is © The Royal Society of Chemistry 2014

```
   15  H    0.000000
   16  C    0.056080
   17  H    0.000000
   18  C   -0.106570
   19  C   -0.062827
   20  C    0.047868
   21  H    0.000000
   22  C    0.014508
   23  H    0.000000
   24  C    0.000426
   25  H    0.000000
   26  C    0.020050
   27  H    0.000000
   28  C    1.074113
   29  C    1.110599
   30  O   -0.744130
   31  O   -0.728467
   32  O   -0.686764
   33  C    0.743095
   34  H    0.000000
   35  O   -0.640813
 Sum of APT charges=   0.00000
 Electronic spatial extent (au):  <R**2>=  5329.3768
 Charge=     0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=     3.2453    Y=    -2.6087    Z=     3.3576  Tot=     5.3489
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=  -131.4188   YY=  -138.3206   ZZ=  -133.1695
   XY=    -8.3249   XZ=   -14.7986   YZ=     3.8567
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=     2.8842   YY=    -4.0177   ZZ=     1.1335
   XY=    -8.3249   XZ=   -14.7986   YZ=     3.8567
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=    46.6973  YYY=   -30.7194  ZZZ=   -30.0902  XYY=     6.3954
  XXY=    -8.5754  XXZ=    39.9798  XZZ=   -14.5221  YZZ=    10.3814
  YYZ=    36.6647  XYZ=     8.4415
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX= -3440.6752 YYYY= -2007.3423 ZZZZ= -1612.0092 XXXY=   -36.0487
 XXXZ=  -119.2983 YYYX=   -94.8950 YYYZ=    28.6651 ZZZX=   -27.0932
 ZZZY=     7.6859 XXYY=  -973.4590 XXZZ=  -899.1875 YYZZ=  -618.3980
 XXYZ=    -7.3236 YYXZ=   -61.7977 ZZXY=     4.9796
 N-N= 1.915619609174D+03 E-N=-6.230932472632D+03  KE=
1.022610964568D+03
  Exact polarizability: 296.561  -1.576 236.708 -18.474   2.874
185.013
 Approx polarizability: 476.427  12.100 468.767 -29.793   7.713
314.776
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
```

1	6	-0.001458548	-0.000605817	0.001691582
2	6	-0.000297444	0.009711325	0.002832480
3	6	-0.000429644	0.000106992	-0.000165971
4	6	0.000463581	0.000215345	-0.000179516
5	1	-0.000162261	0.000497300	-0.000699927
6	6	-0.000074940	0.000314119	0.001155266
7	1	0.000227890	0.000060637	0.000461007
8	6	-0.000823910	-0.001314271	-0.003996366
9	1	0.000226092	0.000682068	0.000793830
10	6	-0.000139167	-0.000256116	0.000361916
11	1	-0.001234113	-0.001072928	0.001079476
12	6	-0.000078630	-0.000195703	-0.000040480
13	1	0.000081204	0.000023843	0.000043171
14	6	-0.000150117	0.000031082	0.000092263
15	1	0.000016350	0.000023448	-0.000024215
16	6	0.000046494	-0.000030891	-0.000055212
17	1	0.000022197	0.000014466	-0.000001233
18	6	-0.000189056	0.000205534	-0.000156767
19	6	0.002671265	-0.001071820	-0.000971050
20	6	0.002669387	0.000093958	0.001850677
21	1	0.002286223	-0.003577248	-0.000059271
22	6	-0.000727439	-0.001086317	0.000332893
23	1	-0.000063936	0.000080121	0.000189942
24	6	0.000159587	-0.000008209	-0.000397289
25	1	-0.000042512	-0.000114337	-0.000022158
26	6	0.000025043	-0.000310804	0.000061506
27	1	-0.000046624	0.000010526	0.000129286
28	6	-0.000847179	-0.000077457	-0.000068619
29	6	-0.000433191	-0.000190286	-0.000095883
30	8	0.000066692	0.000127373	-0.000167385
31	8	0.000228372	0.000241304	0.000072239
32	8	0.000033140	-0.000311050	0.000273563
33	6	0.015377302	-0.005866599	-0.010452087
34	1	-0.005186233	0.003328074	0.001558352
35	8	-0.012215875	0.000322338	0.004573979

Cartesian Forces: Max 0.015377302 RMS 0.002702060

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Internal Forces: Max 0.010285388 RMS 0.001288261
Search for a saddle point.
Step number 1 out of a maximum of 202
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Swaping is turned off.
Second derivative matrix not updated -- analytic derivatives used.
Eigenvalues --- -0.01909 0.00055 0.00370 0.00706
0.00849
Eigenvalues --- 0.01049 0.01255 0.01435 0.01476
0.01523

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.01599   0.01708   0.01755   0.01799
0.01913
     Eigenvalues ---    0.01975   0.02112   0.02175   0.02191
0.02233
     Eigenvalues ---    0.02358   0.02429   0.02449   0.02516
0.02687
     Eigenvalues ---    0.02728   0.02746   0.02753   0.03279
0.03541
     Eigenvalues ---    0.04214   0.05549   0.07043   0.07507
0.07850
     Eigenvalues ---    0.08807   0.10215   0.11075   0.11181
0.11227
     Eigenvalues ---    0.11852   0.12290   0.12500   0.12528
0.12662
     Eigenvalues ---    0.12839   0.13917   0.14302   0.14685
0.16399
     Eigenvalues ---    0.17719   0.18538   0.19086   0.19186
0.19337
     Eigenvalues ---    0.19424   0.20138   0.20431   0.20932
0.21178
     Eigenvalues ---    0.23372   0.23906   0.24419   0.25102
0.26098
     Eigenvalues ---    0.27639   0.27939   0.29120   0.30151
0.30368
     Eigenvalues ---    0.31255   0.33100   0.34004   0.34050
0.35021
     Eigenvalues ---    0.35291   0.35919   0.36086   0.36133
0.36204
     Eigenvalues ---    0.36239   0.36330   0.36537   0.37438
0.37837
     Eigenvalues ---    0.38859   0.39873   0.40323   0.41142
0.42462
     Eigenvalues ---    0.44487   0.46421   0.47306   0.47640
0.50257
     Eigenvalues ---    0.50621   0.79399   0.89039
0.902541000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                          R1        R2        R3        R4        R5
          1            -0.04638   0.02320   0.17745   0.01773
0.41202
                          R6        R7        R8        R9        R10
          1             0.13460  -0.04624  -0.02017  -0.05747
0.17933
                          R11       R12       R13       R14       R15
          1             0.01885  -0.00837   0.41217   0.16257  -
0.05685
                          R16       R17       R18       R19       R20
          1             0.26506  -0.00781  -0.09525   0.17255  -
0.00908
                          R21       R22       R23       R24       R25
          1            -0.03081  -0.00747   0.18321  -0.01055  -
0.02477
                          R26       R27       R28       R29       R30
          1             0.07972  -0.00125  -0.01368   0.00007
0.01491
                          R31       R32       R33       R34       R35
          1            -0.00022  -0.01562  -0.00028   0.02094
0.01768
                          R36       R37       R38       R39       R40
          1             0.01716  -0.00156  -0.01217  -0.03758
0.00008
                          R41       R42       R43       R44       R45
          1             0.01360  -0.00013  -0.01479  -0.00013
0.00379
                          R46       R47       R48       R49       R50
          1             0.00102  -0.00295   0.00259  -0.00060
0.00552
```

This journal is © The Royal Society of Chemistry 2014

	A1	A2	A3	A4	A5
1	0.02038	-0.00825	-0.01181	0.03741	0.01129
	A6	A7	A8	A9	A10
1	0.01809	0.01795	-0.00206	-0.01503	0.02509
	A11	A12	A13	A14	A15
1	0.05204	0.02112	0.05281	0.03312	0.01553
	A16	A17	A18	A19	A20
1	0.05626	0.01464	0.02797	-0.00427	0.00602
	A21	A22	A23	A24	A25
1	-0.00178	-0.00100	0.00462	-0.00362	-0.00163
	A26	A27	A28	A29	A30
1	-0.00076	0.00241	0.00394	-0.00629	0.00231
	A31	A32	A33	A34	A35
1	0.01880	-0.01695	-0.00096	0.02037	-0.00752
	A36	A37	A38	A39	A40
1	-0.01234	-0.00266	0.00624	-0.00360	-0.00118
	A41	A42	A43	A44	A45
1	0.00445	-0.00325	-0.00123	-0.00128	0.00251
	A46	A47	A48	A49	A50
1	0.00396	-0.00616	0.00211	-0.00520	0.00481
	A51	A52	A53	A54	A55
1	0.00043	-0.00432	0.00155	0.00282	-0.01360
	A56	A57	A58	D1	D2
1	-0.00265	0.01000	-0.00746	0.13844	-0.01999
	D3	D4	D5	D6	D7
1	0.13424	-0.02419	0.01063	-0.00061	0.01460
	D8	D9	D10	D11	D12
1	0.00336	0.00214	0.00377	-0.00350	-0.00187
	D13	D14	D15	D16	D17
1	-0.13853	-0.13164	0.01868	0.02558	0.08898
	D18	D19	D20	D21	D22
1	0.09462	-0.07659	-0.07094	0.05150	-0.15532
	D23	D24	D25	D26	D27
1	0.06376	-0.14307	-0.00254	0.00193	-0.01606
	D28	D29	D30	D31	D32

```
          1             -0.01158   0.15503   0.14388  -0.05411  -
0.06527
                           D33       D34       D35       D36       D37
          1             -0.00146   0.17341  -0.17619  -0.00132  -
0.14435
                           D38       D39       D40       D41       D42
          1             -0.14869   0.02614   0.02180  -0.02411  -
0.02018
                           D43       D44       D45       D46       D47
          1              0.14978   0.15371  -0.00171  -0.00077  -
0.00008
                           D48       D49       D50       D51       D52
          1              0.00086  -0.00060   0.00151   0.00035
0.00247
                           D53       D54       D55       D56       D57
          1              0.00016  -0.00443   0.00226  -0.00233  -
0.00990
                           D58       D59       D60       D61       D62
          1             -0.01652  -0.00004  -0.00667   0.01524
0.01018
                           D63       D64       D65       D66       D67
          1              0.00275  -0.00231   0.00134  -0.00283
0.00981
                           D68       D69       D70       D71       D72
          1              0.00564   0.00223  -0.00044  -0.00202  -
0.00468
                           D73       D74       D75       D76       D77
          1              0.00144  -0.00338  -0.00123  -0.00606
0.00222
                           D78       D79       D80       D81       D82
          1              0.00744  -0.00260   0.00261   0.04332
0.03977
                           D83       D84
          1             -0.04433  -0.04045
 RFO step:  Lambda0=1.840677650D-05 Lambda=-3.62631284D-03.
 Linear search not attempted -- option 19 set.
 Maximum step size (   0.300) exceeded in Quadratic search.
    -- Step size scaled by   0.495
 Iteration  1 RMS(Cart)=  0.03374164 RMS(Int)=  0.00089611
 Iteration  2 RMS(Cart)=  0.00106213 RMS(Int)=  0.00012366
 Iteration  3 RMS(Cart)=  0.00000085 RMS(Int)=  0.00012366
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.74906   0.00472   0.00000   0.00438   0.00442
2.75348
    R2        2.68996   0.00098   0.00000   0.00029   0.00034
2.69030
    R3        5.32605   0.00156   0.00000   0.04664   0.04668
5.37273
    R4        2.67465   0.00163   0.00000   0.00110   0.00111
2.67576
```

This journal is © The Royal Society of Chemistry 2014

R5	4.19582	0.00198	0.00000	0.07462	0.07469
4.27051					
R6	4.71349	-0.00057	0.00000	0.03790	0.03793
4.75142					
R7	2.75117	0.00325	0.00000	0.00354	0.00317
2.75435					
R8	2.84755	-0.00431	0.00000	-0.01386	-0.01401
2.83354					
R9	2.71952	-0.00049	0.00000	0.00232	0.00233
2.72185					
R10	5.28847	-0.00025	0.00000	-0.02112	-0.02117
5.26730					
R11	2.66881	0.00002	0.00000	-0.00110	-0.00110
2.66771					
R12	2.05821	0.00026	0.00000	-0.00008	-0.00006
2.05815					
R13	4.11071	-0.00065	0.00000	-0.06385	-0.06386
4.04685					
R14	4.68581	0.00003	0.00000	-0.04512	-0.04508
4.64072					
R15	2.72477	-0.00079	0.00000	0.00279	0.00284
2.72761					
R16	4.94999	-0.00112	0.00000	-0.07460	-0.07464
4.87535					
R17	2.04558	-0.00007	0.00000	0.00067	0.00066
2.04625					
R18	2.67027	-0.00114	0.00000	-0.00117	-0.00117
2.66909					
R19	5.11658	0.00002	0.00000	-0.01994	-0.01986
5.09672					
R20	2.80205	0.00018	0.00000	0.00520	0.00520
2.80725					
R21	5.17898	-0.00013	0.00000	-0.01440	-0.01442
5.16456					
R22	2.04482	0.00049	0.00000	-0.00077	-0.00078
2.04404					
R23	5.17031	0.00175	0.00000	0.05701	0.05692
5.22723					
R24	2.80452	0.00073	0.00000	-0.00312	-0.00311
2.80141					
R25	5.22067	0.00037	0.00000	0.03641	0.03643
5.25709					
R26	5.28767	-0.00132	0.00000	-0.02798	-0.02806
5.25962					
R27	2.04932	-0.00112	0.00000	-0.00059	-0.00059
2.04873					
R28	2.61812	0.00007	0.00000	0.00038	0.00038
2.61850					
R29	2.05321	-0.00002	0.00000	0.00000	0.00000
2.05321					
R30	2.66335	-0.00082	0.00000	-0.00087	-0.00087
2.66248					

This journal is © The Royal Society of Chemistry 2014

R31	2.05293	-0.00003	0.00000	-0.00008	-0.00008
2.05285					
R32	2.61459	-0.00067	0.00000	0.00022	0.00021
2.61481					
R33	2.05387	-0.00002	0.00000	-0.00004	-0.00004
2.05383					
R34	2.68479	0.00036	0.00000	0.00103	0.00092
2.68572					
R35	2.66661	0.00006	0.00000	-0.00138	-0.00138
2.66523					
R36	2.67045	0.00009	0.00000	0.00164	0.00140
2.67185					
R37	2.04830	-0.00063	0.00000	-0.00225	-0.00209
2.04620					
R38	2.62107	0.00022	0.00000	0.00060	0.00059
2.62166					
R39	3.95239	0.00531	0.00000	0.09321	0.09353
4.04592					
R40	2.05360	-0.00004	0.00000	0.00003	0.00003
2.05363					
R41	2.66412	-0.00025	0.00000	-0.00125	-0.00116
2.66296					
R42	2.05358	0.00004	0.00000	0.00000	0.00000
2.05357					
R43	2.61837	-0.00044	0.00000	0.00014	0.00023
2.61860					
R44	2.05532	-0.00001	0.00000	-0.00002	-0.00002
2.05530					
R45	2.64221	-0.00026	0.00000	0.00368	0.00366
2.64587					
R46	2.27339	-0.00033	0.00000	-0.00025	-0.00025
2.27314					
R47	2.64066	-0.00021	0.00000	-0.00481	-0.00483
2.63583					
R48	2.27334	-0.00032	0.00000	-0.00042	-0.00042
2.27292					
R49	2.05948	0.00628	0.00000	0.01026	0.01026
2.06974					
R50	2.31763	-0.01029	0.00000	-0.00578	-0.00571
2.31192					
A1	2.03162	-0.00055	0.00000	0.00019	0.00021
2.03184					
A2	2.18002	0.00281	0.00000	0.00397	0.00389
2.18391					
A3	2.06881	-0.00224	0.00000	-0.00305	-0.00310
2.06571					
A4	2.05033	-0.00152	0.00000	-0.00371	-0.00384
2.04649					
A5	2.06708	0.00240	0.00000	0.00168	0.00169
2.06877					
A6	2.07325	-0.00053	0.00000	0.02069	0.01979
2.09304					

This journal is © The Royal Society of Chemistry 2014

A7	2.03730	0.00090	0.00000	-0.00035	-0.00038
2.03693					
A8	2.09839	0.00101	0.00000	0.00233	0.00233
2.10072					
A9	2.14470	-0.00189	0.00000	-0.00164	-0.00163
2.14307					
A10	2.04914	-0.00034	0.00000	-0.00214	-0.00221
2.04693					
A11	2.06160	0.00035	0.00000	-0.00632	-0.00645
2.05515					
A12	2.05835	-0.00018	0.00000	-0.00193	-0.00198
2.05637					
A13	2.17912	-0.00022	0.00000	-0.00554	-0.00561
2.17351					
A14	2.07172	-0.00002	0.00000	-0.00312	-0.00322
2.06850					
A15	1.86898	0.00037	0.00000	-0.00257	-0.00260
1.86638					
A16	2.18496	-0.00023	0.00000	0.00688	0.00667
2.19163					
A17	1.86519	-0.00031	0.00000	0.00260	0.00255
1.86774					
A18	2.08041	0.00046	0.00000	0.00576	0.00562
2.08603					
A19	2.10228	0.00118	0.00000	0.00343	0.00341
2.10568					
A20	2.10038	0.00083	0.00000	0.00099	0.00099
2.10137					
A21	2.08043	-0.00201	0.00000	-0.00454	-0.00456
2.07588					
A22	2.08593	-0.00028	0.00000	-0.00131	-0.00132
2.08462					
A23	2.10799	0.00045	0.00000	0.00107	0.00108
2.10907					
A24	2.08921	-0.00017	0.00000	0.00028	0.00027
2.08948					
A25	2.09257	0.00022	0.00000	0.00081	0.00081
2.09338					
A26	2.09484	-0.00045	0.00000	-0.00143	-0.00144
2.09340					
A27	2.09574	0.00024	0.00000	0.00066	0.00066
2.09640					
A28	2.09499	0.00040	0.00000	0.00021	0.00020
2.09519					
A29	2.08221	-0.00022	0.00000	-0.00038	-0.00038
2.08184					
A30	2.10593	-0.00019	0.00000	0.00014	0.00015
2.10608					
A31	2.03588	0.00067	0.00000	0.00117	0.00110
2.03698					
A32	2.14799	-0.00130	0.00000	-0.00406	-0.00388
2.14411					

This journal is © The Royal Society of Chemistry 2014

A33	2.09558	0.00063	0.00000	0.00297	0.00285
2.09843					
A34	2.03378	0.00026	0.00000	-0.00161	-0.00142
2.03236					
A35	2.17062	0.00065	0.00000	0.00568	0.00518
2.17580					
A36	2.07597	-0.00089	0.00000	-0.00316	-0.00292
2.07305					
A37	2.07743	-0.00168	0.00000	0.00277	0.00253
2.07997					
A38	2.09705	0.00016	0.00000	-0.00021	-0.00027
2.09678					
A39	2.10868	0.00153	0.00000	-0.00256	-0.00226
2.10642					
A40	2.08741	-0.00034	0.00000	-0.00206	-0.00203
2.08538					
A41	2.10666	0.00045	0.00000	0.00222	0.00216
2.10882					
A42	2.08910	-0.00011	0.00000	-0.00016	-0.00013
2.08897					
A43	2.09287	0.00030	0.00000	0.00096	0.00094
2.09381					
A44	2.09514	-0.00037	0.00000	-0.00154	-0.00151
2.09364					
A45	2.09517	0.00007	0.00000	0.00058	0.00057
2.09574					
A46	2.09508	0.00002	0.00000	-0.00031	-0.00035
2.09473					
A47	2.08389	-0.00007	0.00000	-0.00023	-0.00021
2.08368					
A48	2.10404	0.00005	0.00000	0.00049	0.00051
2.10455					
A49	1.88671	0.00018	0.00000	-0.00070	-0.00069
1.88602					
A50	2.27607	-0.00001	0.00000	0.00275	0.00275
2.27881					
A51	2.12035	-0.00016	0.00000	-0.00202	-0.00202
2.11833					
A52	1.88542	-0.00001	0.00000	0.00041	0.00041
1.88583					
A53	2.27408	-0.00009	0.00000	-0.00324	-0.00324
2.27084					
A54	2.12361	0.00010	0.00000	0.00280	0.00280
2.12641					
A55	1.90661	-0.00022	0.00000	0.00042	0.00040
1.90700					
A56	2.05282	-0.00170	0.00000	-0.01527	-0.01513
2.03769					
A57	2.14374	0.00307	0.00000	0.01640	0.01591
2.15966					
A58	2.08640	-0.00136	0.00000	-0.00156	-0.00142
2.08498					

This journal is © The Royal Society of Chemistry 2014

D1	-0.59147	0.00062	0.00000	-0.00686	-0.00688	-0.59836
D2	3.00378	-0.00002	0.00000	-0.05522	-0.05469	2.94909
D3	2.63087	0.00045	0.00000	-0.02305	-0.02319	2.60768
D4	-0.05706	-0.00019	0.00000	-0.07142	-0.07100	-0.12806
D5	0.00653	0.00027	0.00000	-0.00054	-0.00049	0.00604
D6	-3.05712	0.00001	0.00000	-0.00513	-0.00514	-3.06226
D7	3.07276	0.00066	0.00000	0.01491	0.01499	3.08775
D8	0.00911	0.00041	0.00000	0.01032	0.01035	0.01945
D9	-0.06995	-0.00015	0.00000	-0.00307	-0.00302	-0.07297
D10	3.08626	-0.00010	0.00000	0.00675	0.00681	3.09307
D11	-3.12921	-0.00040	0.00000	-0.01972	-0.01977	3.13420
D12	0.02700	-0.00035	0.00000	-0.00990	-0.00994	0.01706
D13	0.58174	-0.00075	0.00000	0.00225	0.00226	0.58400
D14	-2.64155	-0.00064	0.00000	0.01533	0.01531	-2.62623
D15	-3.01516	0.00068	0.00000	0.04569	0.04583	-2.96933
D16	0.04474	0.00079	0.00000	0.05877	0.05888	0.10362
D17	-0.04844	-0.00067	0.00000	-0.07593	-0.07581	-0.12425
D18	3.11618	-0.00079	0.00000	-0.05379	-0.05383	3.06235
D19	-2.73034	-0.00108	0.00000	-0.11845	-0.11857	-2.84891
D20	0.43428	-0.00119	0.00000	-0.09631	-0.09659	0.33769
D21	-3.05175	-0.00030	0.00000	-0.01082	-0.01086	-3.06261
D22	0.59431	0.00012	0.00000	0.01095	0.01086	0.60517
D23	0.00965	0.00011	0.00000	-0.00591	-0.00590	0.00375
D24	-2.62748	0.00053	0.00000	0.01587	0.01583	-2.61165
D25	-0.03863	-0.00019	0.00000	-0.00354	-0.00355	-0.04218
D26	3.11329	0.00000	0.00000	-0.00064	-0.00063	3.11266

This journal is © The Royal Society of Chemistry 2014

D27	-3.09731	-0.00061	0.00000	-0.00850	-0.00856	-3.10587
D28	0.05461	-0.00041	0.00000	-0.00559	-0.00564	0.04896
D29	-0.60438	-0.00045	0.00000	-0.01554	-0.01552	-0.61990
D30	2.63015	-0.00052	0.00000	-0.01667	-0.01659	2.61356
D31	3.04435	0.00001	0.00000	0.00642	0.00640	3.05075
D32	-0.00430	-0.00006	0.00000	0.00530	0.00533	0.00103
D33	-0.01125	0.00025	0.00000	-0.03373	-0.03374	-0.04499
D34	2.55234	0.00028	0.00000	-0.00614	-0.00609	2.54625
D35	-2.55451	0.00001	0.00000	-0.01451	-0.01456	-2.56907
D36	0.00908	0.00004	0.00000	0.01309	0.01309	0.02217
D37	-2.68081	-0.00016	0.00000	0.00878	0.00877	-2.67204
D38	0.47408	-0.00007	0.00000	0.01153	0.01152	0.48560
D39	-0.09424	-0.00002	0.00000	-0.01004	-0.01003	-0.10427
D40	3.06065	0.00006	0.00000	-0.00729	-0.00728	3.05337
D41	0.07900	-0.00004	0.00000	-0.01222	-0.01223	0.06677
D42	-3.07425	-0.00008	0.00000	-0.00839	-0.00840	-3.08265
D43	2.68366	-0.00026	0.00000	0.01393	0.01392	2.69758
D44	-0.46960	-0.00030	0.00000	0.01775	0.01776	-0.45184
D45	3.11849	0.00002	0.00000	-0.00147	-0.00144	3.11705
D46	-0.03419	0.00005	0.00000	0.00270	0.00273	-0.03146
D47	-0.00866	0.00004	0.00000	0.00816	0.00816	-0.00051
D48	3.12183	0.00007	0.00000	0.01233	0.01233	3.13416
D49	-3.12807	-0.00003	0.00000	-0.00047	-0.00049	-3.12855
D50	0.00436	0.00016	0.00000	0.00431	0.00432	0.00868
D51	0.00241	0.00000	0.00000	0.00369	0.00369	0.00610
D52	3.13484	0.00019	0.00000	0.00847	0.00849	-3.13986

This journal is © The Royal Society of Chemistry 2014

D53	0.03199	-0.00011	0.00000	-0.00387	-0.00390	0.02810
D54	-3.12007	-0.00031	0.00000	-0.00682	-0.00686	-3.12693
D55	-3.11878	0.00008	0.00000	0.00092	0.00091	-3.11787
D56	0.01234	-0.00012	0.00000	-0.00203	-0.00205	0.01029
D57	0.01230	0.00021	0.00000	0.00846	0.00847	0.02077
D58	-3.05225	0.00003	0.00000	-0.00430	-0.00418	-3.05642
D59	3.06390	0.00017	0.00000	0.00916	0.00912	3.07303
D60	-0.00064	-0.00001	0.00000	-0.00361	-0.00352	-0.00416
D61	3.07742	0.00010	0.00000	0.00377	0.00367	3.08109
D62	-0.08421	0.00002	0.00000	0.00136	0.00129	-0.08291
D63	0.03182	0.00003	0.00000	0.00272	0.00268	0.03450
D64	-3.12981	-0.00005	0.00000	0.00031	0.00030	-3.12951
D65	0.05768	-0.00084	0.00000	-0.01256	-0.01261	0.04507
D66	-3.09002	-0.00021	0.00000	-0.01176	-0.01180	-3.10182
D67	3.11574	-0.00068	0.00000	0.00089	0.00080	3.11654
D68	-0.03196	-0.00005	0.00000	0.00169	0.00161	-0.03035
D69	-3.11350	-0.00006	0.00000	0.00159	0.00160	-3.11190
D70	0.03389	0.00011	0.00000	0.00122	0.00122	0.03511
D71	0.02187	0.00057	0.00000	0.00242	0.00244	0.02432
D72	-3.11393	0.00074	0.00000	0.00205	0.00207	-3.11186
D73	3.13709	-0.00006	0.00000	-0.00047	-0.00047	3.13661
D74	-0.00238	-0.00008	0.00000	-0.00214	-0.00211	-0.00449
D75	0.00129	0.00011	0.00000	-0.00084	-0.00084	0.00045
D76	-3.13818	0.00009	0.00000	-0.00251	-0.00247	-3.14065
D77	-0.03046	0.00002	0.00000	0.00018	0.00017	-0.03030
D78	3.13140	0.00011	0.00000	0.00263	0.00258	3.13398

```
   D79        3.11325   0.00000   0.00000  -0.00148  -0.00147
3.11179
   D80       -0.00807   0.00009   0.00000   0.00097   0.00095  -
0.00712
   D81       -0.14061   0.00004   0.00000   0.00587   0.00587  -
0.13475
   D82        3.01139   0.00007   0.00000   0.00242   0.00242
3.01381
   D83        0.14616  -0.00003   0.00000   0.00232   0.00232
0.14848
   D84       -3.00735  -0.00011   0.00000  -0.00020  -0.00020  -
3.00755
         Item               Value     Threshold  Converged?
 Maximum Force            0.010285     0.000450     NO
 RMS     Force            0.001288     0.000300     NO
 Maximum Displacement     0.237732     0.001800     NO
 RMS     Displacement     0.033722     0.001200     NO
 Predicted change in Energy=-1.505845D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.572655    0.502775    1.145612
    2          6             0        0.572827    1.052108    0.432043
    3          6             0       -0.743484   -0.908957    1.077855
    4          6             0        0.235943   -1.643873    0.319430
    5          1             0        0.073083   -2.713874    0.197910
    6          6             0       -0.199631   -0.940275   -1.655729
    7          1             0        0.503650   -1.619168   -2.121575
    8          6             0       -0.072654    0.466426   -1.652968
    9          1             0        0.751755    1.024612   -2.075775
   10          6             0       -1.551573    1.266763    1.826025
   11          1             0       -1.454913    2.343618    1.906009
   12          6             0       -2.634713    0.644431    2.425636
   13          1             0       -3.364462    1.243515    2.963293
   14          6             0       -2.804481   -0.751555    2.339224
   15          1             0       -3.665557   -1.222871    2.804527
   16          6             0       -1.876874   -1.519211    1.657416
   17          1             0       -2.003338   -2.595269    1.571824
   18          6             0        1.598474   -1.168073    0.341548
   19          6             0        1.782598    0.240459    0.386263
   20          6             0        3.095701    0.758195    0.303939
   21          1             0        3.241625    1.831077    0.313770
   22          6             0        4.179907   -0.103095    0.218246
   23          1             0        5.186248    0.305633    0.183473
   24          6             0        3.991344   -1.498742    0.169319
   25          1             0        4.850436   -2.160360    0.097583
```

26	6	0	2.710524	-2.025843	0.212157
27	1	0	2.552876	-3.101067	0.167946
28	6	0	-1.443876	1.025861	-1.719373
29	6	0	-1.650441	-1.243612	-1.755442
30	8	0	-2.350397	-0.040093	-1.671020
31	8	0	-2.215197	-2.299203	-1.871454
32	8	0	-1.820967	2.165693	-1.793815
33	6	0	0.662463	2.538709	0.257920
34	1	0	-0.205891	3.125568	0.575956
35	8	0	1.618116	3.106628	-0.252902

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.457077	0.000000			
3	C	1.423644	2.448575	0.000000		
4	C	2.438135	2.719280	1.440342	0.000000	
5	H	3.414960	3.806204	2.167674	1.089125	0.000000
6	C	3.173177	2.987486	2.787335	2.141501	2.579924
7	H	4.041731	3.696143	3.506579	2.455766	2.600727
8	C	2.843127	2.259854	3.130348	2.904986	3.682567
9	H	3.521890	2.514343	3.989963	3.622690	4.427925
10	C	1.415952	2.549968	2.438549	3.733208	4.597362
11	H	2.178368	2.819983	3.430920	4.612625	5.552531
12	C	2.431175	3.798542	2.793971	4.232387	4.855217
13	H	3.412748	4.684667	3.880404	5.318828	5.926634
14	C	2.824731	4.277470	2.421474	3.757655	4.088557
15	H	3.910997	5.363590	3.408584	4.644852	4.795307
16	C	2.459951	3.756894	1.411692	2.503945	2.712878
17	H	3.438952	4.608588	2.162149	2.736425	2.492635
18	C	2.855180	2.447314	2.468614	1.443387	2.176454
19	C	2.488501	1.457537	2.860165	2.438712	3.418480
20	C	3.772332	2.543166	4.256488	3.734754	4.604642
21	H	4.123722	2.782673	4.896193	4.594501	5.541631
22	C	4.879952	3.793577	5.062422	4.235456	4.866476
23	H	5.842050	4.680029	6.118568	5.322085	5.938190
24	C	5.078317	4.273420	4.857148	3.761202	4.102455
25	H	6.131930	5.360014	5.815401	4.648605	4.810358
26	C	4.247883	3.753915	3.731895	2.506185	2.725745
27	H	4.869544	4.608601	4.061930	2.741267	2.510018
28	C	3.039866	2.948961	3.472542	3.755794	4.467970
29	C	3.553535	3.872770	2.993683	2.832622	2.991286
30	O	3.374684	3.763113	3.300516	3.636366	4.063897
31	O	4.433026	4.930564	3.577310	3.352241	3.112948
32	O	3.600529	3.453225	4.342916	4.817621	5.600408
33	C	2.541366	1.499445	3.812529	4.204723	5.285887
34	H	2.708887	2.219538	4.101012	4.796727	5.858313
35	O	3.679044	2.404752	4.844893	4.980484	6.038924

		6	7	8	9	10
6	C	0.000000				
7	H	1.082827	0.000000			
8	C	1.412422	2.213915	0.000000		

This journal is © The Royal Society of Chemistry 2014

9	H	2.223141	2.655792	1.081660	0.000000	
10	C	4.338361	5.304346	3.864083	4.537400	0.000000
11	H	5.004564	5.980057	4.254505	4.739595	1.084139
12	C	5.009836	5.970790	4.819838	5.645830	1.385649
13	H	6.010030	7.000938	5.722738	6.510251	2.140207
14	C	4.772893	5.620962	4.988382	5.940859	2.430383
15	H	5.655650	6.465742	5.969249	6.955657	3.409497
16	C	3.758356	4.467400	4.261056	5.226608	2.809964
17	H	4.050860	4.569350	4.847762	5.830871	3.896666
18	C	2.697070	2.732965	3.072840	3.371683	4.249105
19	C	3.081087	3.373896	2.766131	2.781935	3.773978
20	C	4.193366	4.272435	3.735384	3.350836	4.916558
21	H	4.837516	5.033051	4.088371	3.543975	5.057679
22	C	4.836632	4.613903	4.680819	4.276269	6.108299
23	H	5.826032	5.562808	5.572649	5.028505	7.001427
24	C	4.605102	4.174531	4.868130	4.680032	6.412224
25	H	5.483237	4.910407	5.848183	5.627319	7.464476
26	C	3.624426	3.237589	4.175665	4.286803	5.622392
27	H	3.946025	3.411343	4.789169	5.029866	6.218816
28	C	2.327635	3.309200	1.482440	2.224370	3.555205
29	C	1.485532	2.217027	2.328979	3.319338	4.374776
30	O	2.331599	3.292729	2.333453	3.304660	3.817764
31	O	2.440436	2.813741	3.505272	4.460078	5.179563
32	O	3.506399	4.453812	2.442119	2.828510	3.739504
33	C	4.063076	4.793241	2.913117	2.783270	2.996457
34	H	4.638053	5.503876	3.472304	3.516074	2.613176
35	O	4.652907	5.202607	3.433592	2.899696	4.213546

		11	12	13	14	15
11	H	0.000000				
12	C	2.132880	0.000000			
13	H	2.444270	1.086513	0.000000		
14	C	3.404278	1.408924	2.164105	0.000000	
15	H	4.291168	2.166337	2.489764	1.086322	0.000000
16	C	3.893751	2.417815	3.398660	1.383695	2.145476
17	H	4.980468	3.409294	4.304081	2.151747	2.483144
18	C	4.909449	5.054549	6.109013	4.852856	5.811995
19	C	4.149022	4.882097	5.842896	5.083251	6.137730
20	C	5.078217	6.111644	7.002957	6.421362	7.476107
21	H	4.985519	6.356057	7.141820	6.879525	7.952335
22	C	6.370725	7.202111	8.140402	7.328078	8.336309
23	H	7.157202	8.143065	9.040004	8.343661	9.357388
24	C	6.887782	7.320436	8.332716	7.172867	8.102380
25	H	7.956988	8.325511	9.342549	8.099842	8.984908
26	C	6.269943	6.371923	7.427174	6.046776	6.929614
27	H	6.980533	6.785057	7.855205	6.239866	7.010570
28	C	3.857461	4.329513	5.065904	4.634939	5.518906
29	C	5.129589	4.692005	5.602690	4.282548	4.985422
30	O	4.390799	4.163172	4.914554	4.098101	4.812393
31	O	6.033494	5.225511	6.102987	4.524630	5.012667
32	O	3.722144	4.558529	5.085554	5.153605	6.002468
33	C	2.690267	4.377059	5.021224	5.213192	6.274269
34	H	1.985080	3.934023	4.383842	4.989376	5.987048

This journal is © The Royal Society of Chemistry 2014

35	O	3.832308	5.596743	6.216203	6.415923	7.483958
		16	17	18	19	20
16	C	0.000000				
17	H	1.086840	0.000000			
18	C	3.732673	4.064913	0.000000		
19	C	4.254880	4.876497	1.421220	0.000000	
20	C	5.634268	6.233254	2.440003	1.413884	0.000000
21	H	6.263294	6.977455	3.419886	2.159649	1.082805
22	C	6.384449	6.802619	2.795206	2.427622	1.387323
23	H	7.442463	7.876097	3.881871	3.410309	2.142361
24	C	6.053993	6.253448	2.421742	2.819654	2.431884
25	H	6.935478	7.024013	3.408726	3.906264	3.411692
26	C	4.836287	4.938971	1.410378	2.455094	2.812055
27	H	4.933911	4.794350	2.162750	3.436101	3.899623
28	C	4.250597	4.925196	4.279794	3.932009	4.977269
29	C	3.431446	3.608630	3.867625	4.309887	5.547446
30	O	3.672942	4.143117	4.573440	4.625232	5.847882
31	O	3.629845	3.462471	4.552023	5.246860	6.502743
32	O	5.049023	5.833313	5.231285	4.630868	5.527681
33	C	4.987337	5.932164	3.824048	2.559907	3.015460
34	H	5.053287	6.078697	4.663265	3.509120	4.071727
35	O	6.104314	6.996870	4.315881	2.941174	2.829924
		21	22	23	24	25
21	H	0.000000				
22	C	2.151864	0.000000			
23	H	2.474978	1.086734	0.000000		
24	C	3.416231	1.409177	2.164201	0.000000	
25	H	4.308895	2.167143	2.490235	1.086703	0.000000
26	C	3.894641	2.419934	3.400855	1.385702	2.147195
27	H	4.982137	3.411392	4.305868	2.153286	2.483679
28	C	5.170684	6.054407	6.935280	6.283502	7.285032
29	C	6.137399	6.260126	7.273230	5.966535	6.821696
30	O	6.221848	6.798395	7.769151	6.762558	7.712035
31	O	7.184103	7.077223	8.111060	6.582298	7.336181
32	O	5.493972	6.723561	7.514689	7.145974	8.173111
33	C	2.675059	4.399217	5.045474	5.233575	6.296513
34	H	3.691858	5.457788	6.097643	6.258305	7.330506
35	O	2.141011	4.133651	4.557144	5.198068	6.189660
		26	27	28	29	30
26	C	0.000000				
27	H	1.087619	0.000000			
28	C	5.504793	6.047110	0.000000		
29	C	4.847819	4.981711	2.279140	0.000000	
30	O	5.753476	6.065761	1.400134	1.394820	0.000000
31	O	5.355268	5.247539	3.416740	1.202780	2.272010
32	O	6.490555	7.121641	1.202895	3.413782	2.271754
33	C	5.003177	5.948852	3.261144	4.869200	4.410030
34	H	5.930840	6.822629	3.348121	5.158670	4.435000
35	O	5.268006	6.291770	3.981950	5.644970	5.259469
		31	32	33	34	35
31	O	0.000000				
32	O	4.482938	0.000000			

```
   33  C    6.018352   3.242867   0.000000
   34  H    6.281343   3.024177   1.095258   0.000000
   35  O    6.821804   3.884207   1.223415   2.003588   0.000000
 Stoichiometry    C19H12O4
 Framework group  C1[X(C19H12O4)]
 Deg. of freedom    99
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6              0       -0.563311    0.531048    1.138196
    2          6              0        0.577257    1.061231    0.402612
    3          6              0       -0.736132   -0.881712    1.106530
    4          6              0        0.236698   -1.636287    0.358997
    5          1              0        0.071794   -2.708753    0.265109
    6          6              0       -0.213224   -0.980990   -1.629516
    7          1              0        0.485765   -1.672015   -2.083844
    8          6              0       -0.084756    0.425194   -1.662366
    9          1              0        0.736981    0.971784   -2.105058
   10          6              0       -1.536199    1.312763    1.807024
   11          1              0       -1.437803    2.391141    1.859725
   12          6              0       -2.615375    0.706720    2.430011
   13          1              0       -3.340365    1.319760    2.958293
   14          6              0       -2.787261   -0.690760    2.379300
   15          1              0       -3.645248   -1.149413    2.862613
   16          6              0       -1.865697   -1.476113    1.709559
   17          1              0       -1.993939   -2.553795    1.651460
   18          6              0        1.599856   -1.161770    0.359013
   19          6              0        1.785792    0.247208    0.367622
   20          6              0        3.098769    0.761137    0.262575
   21          1              0        3.245888    1.833756    0.244869
   22          6              0        4.181385   -0.103340    0.189865
   23          1              0        5.187859    0.303165    0.137373
   24          6              0        3.990993   -1.499534    0.176761
   25          1              0        4.848818   -2.163778    0.114800
   26          6              0        2.709986   -2.023838    0.242321
   27          1              0        2.550879   -3.099630    0.225805
   28          6              0       -1.455859    0.984518   -1.732084
   29          6              0       -1.665071   -1.284898   -1.710676
   30          8              0       -2.363100   -0.078802   -1.650592
   31          8              0       -2.231802   -2.342327   -1.796353
   32          8              0       -1.832314    2.122636   -1.831700
   33          6              0        0.667116    2.542983    0.191253
   34          1              0       -0.198166    3.138567    0.501343
   35          8              0        1.619431    3.096973   -0.340664
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3952724      0.2612382
0.2440496
```

This journal is © The Royal Society of Chemistry 2014

```
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1913.2030981941 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1032.13656396     A.U. after   15 cycles
            Convg  =    0.7938D-08             -V/T =  2.0093
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000884493   -0.000406649    0.001050923
    2          6          -0.000252334    0.004987264    0.002547837
    3          6          -0.000306781    0.000136932   -0.000115923
    4          6           0.000148116    0.000117335   -0.000697587
    5          1          -0.000058604    0.000416907   -0.000442604
    6          6           0.000142033   -0.000340947    0.001489515
    7          1           0.000083920    0.000071844    0.000291227
    8          6          -0.000733267   -0.000498493   -0.002938081
    9          1           0.000157906    0.000473600    0.000372509
   10          6           0.000119588   -0.000093582    0.000172517
   11          1          -0.000531889   -0.000478973    0.000499465
   12          6          -0.000074513   -0.000118701    0.000007267
   13          1           0.000043781    0.000010275    0.000028784
   14          6          -0.000078069    0.000044904    0.000079655
   15          1          -0.000000879    0.000016680   -0.000022736
   16          6           0.000075617   -0.000042393   -0.000028622
   17          1           0.000009226    0.000007813    0.000006666
   18          6          -0.000069747    0.000052186   -0.000155253
   19          6           0.001592102   -0.000659466   -0.000757750
   20          6           0.001453325   -0.000029847    0.001103616
   21          1           0.001535618   -0.002088491    0.000043218
   22          6          -0.000387678   -0.000586500    0.000156833
   23          1          -0.000031591    0.000035661    0.000115957
   24          6           0.000082020    0.000019235   -0.000203243
   25          1          -0.000023713   -0.000060115   -0.000009754
   26          6           0.000018103   -0.000141764    0.000053302
   27          1          -0.000026603    0.000005423    0.000059164
   28          6          -0.000401024    0.000037638    0.000020129
   29          6          -0.000239942   -0.000089031   -0.000079378
   30          8           0.000035550    0.000040617   -0.000088696
   31          8           0.000102007    0.000111936    0.000023868
```

```
   32          8           0.000003843   -0.000138620    0.000144376
   33          6           0.008175974   -0.002889182   -0.005345572
   34          1          -0.003133005    0.001590837    0.000349579
   35          8          -0.006544598    0.000485667    0.002268790
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.008175974 RMS     0.001469130


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.005162407 RMS     0.000672381
 Search for a saddle point.
 Step number   2 out of a maximum of 202
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Update second derivatives using D2CorX and points  1  2
     Eigenvalues ---   -0.01913   0.00077   0.00370   0.00709
0.00851
     Eigenvalues ---    0.01046   0.01255   0.01435   0.01473
0.01522
     Eigenvalues ---    0.01600   0.01706   0.01756   0.01799
0.01913
     Eigenvalues ---    0.01975   0.02111   0.02175   0.02191
0.02233
     Eigenvalues ---    0.02358   0.02428   0.02449   0.02516
0.02687
     Eigenvalues ---    0.02727   0.02746   0.02753   0.03269
0.03539
     Eigenvalues ---    0.04208   0.05548   0.07043   0.07506
0.07842
     Eigenvalues ---    0.08806   0.10213   0.11074   0.11181
0.11227
     Eigenvalues ---    0.11852   0.12290   0.12500   0.12528
0.12662
     Eigenvalues ---    0.12839   0.13917   0.14298   0.14683
0.16398
     Eigenvalues ---    0.17714   0.18534   0.19087   0.19185
0.19337
     Eigenvalues ---    0.19423   0.20136   0.20432   0.20928
0.21177
     Eigenvalues ---    0.23371   0.23906   0.24418   0.25102
0.26094
     Eigenvalues ---    0.27638   0.27938   0.29120   0.30151
0.30365
     Eigenvalues ---    0.31254   0.33099   0.34003   0.34049
0.35020
     Eigenvalues ---    0.35289   0.35919   0.36086   0.36133
0.36203
     Eigenvalues ---    0.36239   0.36330   0.36537   0.37437
0.37836
```

```
     Eigenvalues ---    0.38858   0.39873   0.40323   0.41140
0.42462
     Eigenvalues ---    0.44487   0.46424   0.47306   0.47640
0.50257
     Eigenvalues ---    0.50621   0.79400   0.89039
0.902541000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
        1            -0.04559   0.02322   0.17418   0.01783
0.40688
                           R6        R7        R8        R9        R10
        1             0.13098  -0.04561  -0.02023  -0.05815
0.18068
                           R11       R12       R13       R14       R15
```

This journal is © The Royal Society of Chemistry 2014

	1	0.01895	-0.00818	0.41668	0.16545	-0.05733
		R16	R17	R18	R19	R20
	1	0.26869	-0.00776	-0.09493	0.17406	-0.00967
		R21	R22	R23	R24	R25
	1	-0.03089	-0.00732	0.17931	-0.00990	-0.02627
		R26	R27	R28	R29	R30
	1	0.08122	-0.00129	-0.01373	0.00007	0.01477
		R31	R32	R33	R34	R35
	1	-0.00022	-0.01576	-0.00028	0.02093	0.01779
		R36	R37	R38	R39	R40
	1	0.01733	-0.00162	-0.01222	-0.04159	0.00008
		R41	R42	R43	R44	R45
	1	0.01346	-0.00013	-0.01497	-0.00013	0.00361
		R46	R47	R48	R49	R50
	1	0.00100	-0.00295	0.00260	-0.00075	0.00543
		A1	A2	A3	A4	A5
	1	0.02121	-0.00884	-0.01219	0.03680	0.00787
		A6	A7	A8	A9	A10
	1	0.01413	0.01830	-0.00195	-0.01555	0.02692
		A11	A12	A13	A14	A15
	1	0.05341	0.02304	0.05441	0.03458	0.01682
		A16	A17	A18	A19	A20
	1	0.05437	0.01314	0.02532	-0.00426	0.00629
		A21	A22	A23	A24	A25
	1	-0.00205	-0.00102	0.00463	-0.00360	-0.00157
		A26	A27	A28	A29	A30
	1	-0.00090	0.00248	0.00405	-0.00638	0.00228
		A31	A32	A33	A34	A35
	1	0.01922	-0.01746	-0.00089	0.02120	-0.00813
		A36	A37	A38	A39	A40
	1	-0.01270	-0.00283	0.00651	-0.00370	-0.00115
		A41	A42	A43	A44	A45
	1	0.00441	-0.00325	-0.00119	-0.00136	0.00256
		A46	A47	A48	A49	A50

This journal is © The Royal Society of Chemistry 2014

1	0.00408	-0.00623	0.00205	-0.00458	0.00433

	A51	A52	A53	A54	A55
1	0.00027	-0.00473	0.00191	0.00288	-0.01366

	A56	A57	A58	D1	D2
1	-0.00210	0.00965	-0.00772	0.13815	-0.01659

	D3	D4	D5	D6	D7
1	0.13513	-0.01961	0.01144	0.00016	0.01426

	D8	D9	D10	D11	D12
1	0.00299	0.00172	0.00275	-0.00248	-0.00145

	D13	D14	D15	D16	D17
1	-0.13826	-0.13223	0.01731	0.02334	0.09471

	D18	D19	D20	D21	D22
1	0.09954	-0.06957	-0.06474	0.05175	-0.15517

	D23	D24	D25	D26	D27
1	0.06400	-0.14293	-0.00254	0.00192	-0.01602

	D28	D29	D30	D31	D32
1	-0.01156	0.15487	0.14392	-0.05443	-0.06538

	D33	D34	D35	D36	D37
1	-0.00038	0.17348	-0.17552	-0.00166	-0.14497

	D38	D39	D40	D41	D42
1	-0.14928	0.02650	0.02219	-0.02371	-0.01996

	D43	D44	D45	D46	D47
1	0.14883	0.15258	-0.00160	-0.00094	-0.00055

	D48	D49	D50	D51	D52
1	0.00011	-0.00054	0.00143	0.00013	0.00210

	D53	D54	D55	D56	D57
1	0.00034	-0.00425	0.00231	-0.00228	-0.01027

	D58	D59	D60	D61	D62
1	-0.01601	-0.00059	-0.00633	0.01491	0.00996

	D63	D64	D65	D66	D67
1	0.00261	-0.00234	0.00197	-0.00204	0.00936

	D68	D69	D70	D71	D72
1	0.00535	0.00215	-0.00036	-0.00192	-0.00444

	D73	D74	D75	D76	D77

This journal is © The Royal Society of Chemistry 2014

```
         1              0.00139  -0.00329  -0.00114  -0.00582
0.00216
                          D78       D79       D80       D81       D82
         1              0.00727  -0.00253   0.00259   0.04299
0.03962
                          D83       D84
         1             -0.04463  -0.04075
 RFO step:  Lambda0=7.821604377D-07 Lambda=-2.23660996D-03.
 Linear search not attempted -- option 19 set.
 Maximum step size (   0.300) exceeded in Quadratic search.
    -- Step size scaled by   0.437
 Iteration  1 RMS(Cart)=  0.03056575 RMS(Int)=  0.00114767
 Iteration  2 RMS(Cart)=  0.00134881 RMS(Int)=  0.00016233
 Iteration  3 RMS(Cart)=  0.00000162 RMS(Int)=  0.00016233
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00016233
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.75348   0.00224   0.00000  -0.00004  -0.00001
2.75347
    R2        2.69030   0.00037   0.00000  -0.00010  -0.00003
2.69027
    R3        5.37273   0.00090   0.00000   0.04654   0.04658
5.41931
    R4        2.67576   0.00065   0.00000   0.00071   0.00072
2.67648
    R5        4.27051   0.00112   0.00000   0.07965   0.07977
4.35027
    R6        4.75142  -0.00012   0.00000   0.04928   0.04939
4.80081
    R7        2.75435   0.00172   0.00000  -0.00097  -0.00150
2.75284
    R8        2.83354  -0.00214   0.00000  -0.00795  -0.00816
2.82538
    R9        2.72185  -0.00010   0.00000   0.00246   0.00250
2.72436
   R10        5.26730  -0.00020   0.00000  -0.02206  -0.02211
5.24519
   R11        2.66771   0.00000   0.00000  -0.00089  -0.00089
2.66682
   R12        2.05815   0.00007   0.00000  -0.00010  -0.00007
2.05808
   R13        4.04685  -0.00051   0.00000  -0.05703  -0.05706
3.98979
   R14        4.64072  -0.00019   0.00000  -0.04190  -0.04190
4.59883
   R15        2.72761  -0.00027   0.00000   0.00306   0.00315
2.73076
   R16        4.87535  -0.00073   0.00000  -0.06404  -0.06409
4.81126
   R17        2.04625   0.00001   0.00000   0.00056   0.00056
2.04680
```

This journal is © The Royal Society of Chemistry 2014

R18	2.66909	-0.00031	0.00000	-0.00090	-0.00092
2.66817					
R19	5.09672	-0.00002	0.00000	-0.01769	-0.01762
5.07910					
R20	2.80725	0.00012	0.00000	0.00514	0.00514
2.81239					
R21	5.16456	-0.00015	0.00000	-0.00908	-0.00907
5.15549					
R22	2.04404	0.00025	0.00000	-0.00072	-0.00076
2.04328					
R23	5.22723	0.00110	0.00000	0.05340	0.05329
5.28052					
R24	2.80141	0.00037	0.00000	-0.00445	-0.00444
2.79696					
R25	5.25709	0.00035	0.00000	0.03234	0.03235
5.28944					
R26	5.25962	-0.00074	0.00000	-0.00056	-0.00072
5.25890					
R27	2.04873	-0.00049	0.00000	0.00001	0.00001
2.04874					
R28	2.61850	0.00008	0.00000	0.00004	0.00004
2.61854					
R29	2.05321	-0.00001	0.00000	0.00000	0.00000
2.05321					
R30	2.66248	-0.00037	0.00000	-0.00015	-0.00015
2.66233					
R31	2.05285	-0.00002	0.00000	-0.00002	-0.00002
2.05283					
R32	2.61481	-0.00026	0.00000	0.00041	0.00041
2.61521					
R33	2.05383	-0.00001	0.00000	-0.00004	-0.00004
2.05379					
R34	2.68572	0.00019	0.00000	0.00111	0.00096
2.68667					
R35	2.66523	0.00002	0.00000	-0.00112	-0.00111
2.66412					
R36	2.67185	0.00006	0.00000	0.00108	0.00074
2.67259					
R37	2.04620	-0.00027	0.00000	-0.00105	-0.00083
2.04538					
R38	2.62166	0.00011	0.00000	0.00032	0.00032
2.62198					
R39	4.04592	0.00328	0.00000	0.04951	0.04997
4.09589					
R40	2.05363	-0.00002	0.00000	0.00004	0.00004
2.05367					
R41	2.66296	-0.00014	0.00000	-0.00062	-0.00050
2.66246					
R42	2.05357	0.00002	0.00000	0.00001	0.00001
2.05358					
R43	2.61860	-0.00021	0.00000	0.00040	0.00054
2.61914					

This journal is © The Royal Society of Chemistry 2014

R44	2.05530	-0.00001	0.00000	0.00002	0.00002
2.05532					
R45	2.64587	-0.00008	0.00000	0.00390	0.00389
2.64976					
R46	2.27314	-0.00014	0.00000	0.00004	0.00004
2.27318					
R47	2.63583	-0.00007	0.00000	-0.00442	-0.00444
2.63139					
R48	2.27292	-0.00015	0.00000	-0.00031	-0.00031
2.27262					
R49	2.06974	0.00344	0.00000	0.00524	0.00524
2.07498					
R50	2.31192	-0.00516	0.00000	-0.00185	-0.00175
2.31017					
A1	2.03184	-0.00020	0.00000	0.00179	0.00179
2.03363					
A2	2.18391	0.00116	0.00000	-0.00036	-0.00044
2.18347					
A3	2.06571	-0.00095	0.00000	-0.00050	-0.00054
2.06517					
A4	2.04649	-0.00071	0.00000	-0.00075	-0.00083
2.04566					
A5	2.06877	0.00106	0.00000	-0.00110	-0.00090
2.06787					
A6	2.09304	-0.00015	0.00000	0.01859	0.01744
2.11048					
A7	2.03693	0.00040	0.00000	-0.00106	-0.00107
2.03586					
A8	2.10072	0.00045	0.00000	0.00065	0.00065
2.10137					
A9	2.14307	-0.00083	0.00000	0.00061	0.00062
2.14370					
A10	2.04693	-0.00015	0.00000	-0.00189	-0.00193
2.04500					
A11	2.05515	0.00016	0.00000	-0.00538	-0.00548
2.04967					
A12	2.05637	-0.00012	0.00000	-0.00236	-0.00240
2.05397					
A13	2.17351	-0.00013	0.00000	-0.00542	-0.00551
2.16799					
A14	2.06850	-0.00001	0.00000	-0.00347	-0.00357
2.06493					
A15	1.86638	0.00013	0.00000	-0.00334	-0.00337
1.86301					
A16	2.19163	-0.00008	0.00000	0.00573	0.00547
2.19710					
A17	1.86774	-0.00014	0.00000	0.00341	0.00337
1.87112					
A18	2.08603	0.00026	0.00000	0.00577	0.00564
2.09167					
A19	2.10568	0.00053	0.00000	0.00053	0.00051
2.10620					

This journal is © The Royal Society of Chemistry 2014

A20	2.10137	0.00035	0.00000	-0.00007	-0.00007
2.10130					
A21	2.07588	-0.00089	0.00000	-0.00062	-0.00064
2.07524					
A22	2.08462	-0.00012	0.00000	-0.00023	-0.00024
2.08438					
A23	2.10907	0.00019	0.00000	0.00022	0.00022
2.10929					
A24	2.08948	-0.00007	0.00000	0.00004	0.00003
2.08951					
A25	2.09338	0.00010	0.00000	0.00012	0.00012
2.09350					
A26	2.09340	-0.00021	0.00000	-0.00014	-0.00014
2.09326					
A27	2.09640	0.00011	0.00000	0.00003	0.00002
2.09642					
A28	2.09519	0.00016	0.00000	-0.00012	-0.00013
2.09507					
A29	2.08184	-0.00009	0.00000	0.00018	0.00018
2.08202					
A30	2.10608	-0.00008	0.00000	-0.00008	-0.00008
2.10599					
A31	2.03698	0.00032	0.00000	0.00105	0.00095
2.03793					
A32	2.14411	-0.00061	0.00000	-0.00232	-0.00205
2.14206					
A33	2.09843	0.00029	0.00000	0.00128	0.00110
2.09953					
A34	2.03236	0.00007	0.00000	-0.00081	-0.00055
2.03181					
A35	2.17580	0.00036	0.00000	0.00267	0.00200
2.17780					
A36	2.07305	-0.00042	0.00000	-0.00128	-0.00091
2.07213					
A37	2.07997	-0.00091	0.00000	0.00104	0.00071
2.08067					
A38	2.09678	0.00006	0.00000	-0.00049	-0.00059
2.09619					
A39	2.10642	0.00085	0.00000	-0.00056	-0.00013
2.10629					
A40	2.08538	-0.00017	0.00000	-0.00113	-0.00108
2.08430					
A41	2.10882	0.00022	0.00000	0.00129	0.00120
2.11002					
A42	2.08897	-0.00005	0.00000	-0.00016	-0.00011
2.08886					
A43	2.09381	0.00015	0.00000	0.00049	0.00046
2.09427					
A44	2.09364	-0.00017	0.00000	-0.00070	-0.00064
2.09299					
A45	2.09574	0.00003	0.00000	0.00022	0.00019
2.09593					

This journal is © The Royal Society of Chemistry 2014

A46	2.09473	0.00002	0.00000	-0.00012	-0.00018	2.09455
A47	2.08368	-0.00004	0.00000	-0.00001	0.00001	2.08370
A48	2.10455	0.00002	0.00000	0.00011	0.00014	2.10469
A49	1.88602	0.00006	0.00000	-0.00106	-0.00105	1.88497
A50	2.27881	0.00002	0.00000	0.00298	0.00297	2.28179
A51	2.11833	-0.00008	0.00000	-0.00190	-0.00190	2.11642
A52	1.88583	0.00000	0.00000	0.00049	0.00049	1.88632
A53	2.27084	-0.00004	0.00000	-0.00297	-0.00297	2.26787
A54	2.12641	0.00005	0.00000	0.00245	0.00245	2.12887
A55	1.90700	-0.00004	0.00000	0.00021	0.00018	1.90719
A56	2.03769	-0.00105	0.00000	-0.01254	-0.01227	2.02541
A57	2.15966	0.00166	0.00000	0.01181	0.01115	2.17080
A58	2.08498	-0.00059	0.00000	0.00003	0.00030	2.08527
D1	-0.59836	0.00029	0.00000	0.00059	0.00061	-0.59775
D2	2.94909	-0.00021	0.00000	-0.04689	-0.04624	2.90286
D3	2.60768	0.00016	0.00000	-0.01669	-0.01679	2.59089
D4	-0.12806	-0.00034	0.00000	-0.06417	-0.06363	-0.19169
D5	0.00604	0.00012	0.00000	-0.00529	-0.00526	0.00078
D6	-3.06226	-0.00002	0.00000	-0.00833	-0.00838	-3.07063
D7	3.08775	0.00032	0.00000	0.01076	0.01091	3.09866
D8	0.01945	0.00018	0.00000	0.00772	0.00779	0.02724
D9	-0.07297	-0.00005	0.00000	0.00160	0.00165	-0.07132
D10	3.09307	0.00000	0.00000	0.00964	0.00968	3.10275
D11	3.13420	-0.00021	0.00000	-0.01606	-0.01611	3.11809
D12	0.01706	-0.00016	0.00000	-0.00802	-0.00809	0.00897
D13	0.58400	-0.00038	0.00000	-0.00179	-0.00181	0.58219

This journal is © The Royal Society of Chemistry 2014

D14	-2.62623	-0.00028	0.00000	0.00813	0.00805	-2.61818
D15	-2.96933	0.00041	0.00000	0.04153	0.04167	-2.92766
D16	0.10362	0.00051	0.00000	0.05144	0.05153	0.15515
D17	-0.12425	-0.00051	0.00000	-0.09102	-0.09099	-0.21524
D18	3.06235	-0.00072	0.00000	-0.07275	-0.07289	2.98947
D19	-2.84891	-0.00090	0.00000	-0.13505	-0.13510	-2.98401
D20	0.33769	-0.00111	0.00000	-0.11677	-0.11699	0.22070
D21	-3.06261	-0.00017	0.00000	-0.01055	-0.01060	-3.07321
D22	0.60517	0.00010	0.00000	0.00880	0.00869	0.61386
D23	0.00375	0.00003	0.00000	-0.00743	-0.00740	-0.00365
D24	-2.61165	0.00029	0.00000	0.01192	0.01189	-2.59977
D25	-0.04218	-0.00009	0.00000	-0.00224	-0.00226	-0.04444
D26	3.11266	0.00000	0.00000	-0.00009	-0.00008	3.11258
D27	-3.10587	-0.00029	0.00000	-0.00540	-0.00551	-3.11138
D28	0.04896	-0.00019	0.00000	-0.00325	-0.00332	0.04564
D29	-0.61990	-0.00026	0.00000	-0.00988	-0.00984	-0.62974
D30	2.61356	-0.00029	0.00000	-0.01011	-0.01001	2.60355
D31	3.05075	0.00001	0.00000	0.00943	0.00942	3.06016
D32	0.00103	-0.00002	0.00000	0.00920	0.00925	0.01028
D33	-0.04499	-0.00008	0.00000	-0.03716	-0.03715	-0.08214
D34	2.54625	0.00009	0.00000	-0.00842	-0.00836	2.53788
D35	-2.56907	-0.00006	0.00000	-0.01697	-0.01702	-2.58609
D36	0.02217	0.00011	0.00000	0.01177	0.01177	0.03393
D37	-2.67204	-0.00001	0.00000	0.00963	0.00961	-2.66243
D38	0.48560	0.00003	0.00000	0.01130	0.01129	0.49688
D39	-0.10427	-0.00008	0.00000	-0.00994	-0.00993	-0.11419

This journal is © The Royal Society of Chemistry 2014

D40	3.05337	-0.00004	0.00000	-0.00827	-0.00825	3.04512
D41	0.06677	-0.00010	0.00000	-0.01012	-0.01012	0.05665
D42	-3.08265	-0.00011	0.00000	-0.00602	-0.00602	-3.08867
D43	2.69758	-0.00006	0.00000	0.01660	0.01658	2.71416
D44	-0.45184	-0.00007	0.00000	0.02070	0.02069	-0.43115
D45	3.11705	0.00000	0.00000	-0.00072	-0.00070	3.11636
D46	-0.03146	0.00003	0.00000	0.00287	0.00290	-0.02856
D47	-0.00051	0.00003	0.00000	0.00717	0.00717	0.00667
D48	3.13416	0.00006	0.00000	0.01077	0.01077	-3.13825
D49	-3.12855	-0.00001	0.00000	-0.00077	-0.00078	-3.12933
D50	0.00868	0.00008	0.00000	0.00282	0.00284	0.01151
D51	0.00610	0.00001	0.00000	0.00283	0.00283	0.00893
D52	-3.13986	0.00010	0.00000	0.00642	0.00645	-3.13341
D53	0.02810	-0.00006	0.00000	-0.00309	-0.00312	0.02498
D54	-3.12693	-0.00015	0.00000	-0.00528	-0.00533	-3.13226
D55	-3.11787	0.00003	0.00000	0.00050	0.00050	-3.11737
D56	0.01029	-0.00006	0.00000	-0.00169	-0.00171	0.00858
D57	0.02077	0.00015	0.00000	0.00646	0.00647	0.02724
D58	-3.05642	0.00002	0.00000	-0.00301	-0.00288	-3.05930
D59	3.07303	0.00012	0.00000	0.00648	0.00646	3.07949
D60	-0.00416	0.00000	0.00000	-0.00299	-0.00289	-0.00705
D61	3.08109	0.00005	0.00000	0.00225	0.00215	3.08324
D62	-0.08291	0.00000	0.00000	0.00085	0.00078	-0.08213
D63	0.03450	0.00002	0.00000	0.00204	0.00199	0.03649
D64	-3.12951	-0.00002	0.00000	0.00063	0.00062	-3.12889
D65	0.04507	-0.00049	0.00000	-0.00612	-0.00618	0.03889

```
   D66       -3.10182  -0.00015   0.00000  -0.00829  -0.00831  -
3.11013
   D67        3.11654  -0.00037   0.00000   0.00403   0.00391
3.12045
   D68       -0.03035  -0.00003   0.00000   0.00187   0.00178  -
0.02857
   D69       -3.11190  -0.00002   0.00000   0.00151   0.00152  -
3.11038
   D70        0.03511   0.00006   0.00000   0.00026   0.00028
0.03539
   D71        0.02432   0.00032   0.00000  -0.00068  -0.00064
0.02367
   D72       -3.11186   0.00040   0.00000  -0.00193  -0.00188  -
3.11374
   D73        3.13661  -0.00003   0.00000   0.00008   0.00007
3.13669
   D74       -0.00449  -0.00004   0.00000  -0.00127  -0.00123  -
0.00572
   D75        0.00045   0.00005   0.00000  -0.00117  -0.00117  -
0.00072
   D76       -3.14065   0.00005   0.00000  -0.00252  -0.00247
3.14006
   D77       -0.03030   0.00000   0.00000   0.00011   0.00009  -
0.03021
   D78        3.13398   0.00005   0.00000   0.00154   0.00148
3.13546
   D79        3.11179   0.00000   0.00000  -0.00124  -0.00122
3.11057
   D80       -0.00712   0.00004   0.00000   0.00019   0.00017  -
0.00696
   D81       -0.13475   0.00005   0.00000   0.00377   0.00376  -
0.13099
   D82        3.01381   0.00006   0.00000   0.00010   0.00009
3.01390
   D83        0.14848   0.00001   0.00000   0.00363   0.00363
0.15212
   D84       -3.00755  -0.00003   0.00000   0.00207   0.00206  -
3.00549
         Item               Value     Threshold  Converged?
 Maximum Force            0.005162     0.000450     NO
 RMS     Force            0.000672     0.000300     NO
 Maximum Displacement     0.248921     0.001800     NO
 RMS     Displacement     0.030505     0.001200     NO
 Predicted change in Energy=-8.643438D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
```

This journal is © The Royal Society of Chemistry 2014

1	6	0	-0.566608	0.510633	1.149909
2	6	0	0.582019	1.064120	0.444663
3	6	0	-0.744453	-0.899399	1.066871
4	6	0	0.230234	-1.629697	0.295474
5	1	0	0.066358	-2.699230	0.171538
6	6	0	-0.201419	-0.945609	-1.654734
7	1	0	0.500748	-1.624440	-2.123034
8	6	0	-0.080441	0.460973	-1.675920
9	1	0	0.747467	1.019721	-2.090033
10	6	0	-1.532892	1.269516	1.854455
11	1	0	-1.423677	2.342979	1.959906
12	6	0	-2.614723	0.644348	2.453532
13	1	0	-3.333874	1.238974	3.010088
14	6	0	-2.794494	-0.748851	2.346204
15	1	0	-3.654101	-1.222228	2.812106
16	6	0	-1.876007	-1.511822	1.646582
17	1	0	-2.007650	-2.586219	1.549002
18	6	0	1.596191	-1.159575	0.331921
19	6	0	1.787487	0.247967	0.391386
20	6	0	3.104937	0.758187	0.326804
21	1	0	3.258410	1.829334	0.351466
22	6	0	4.184009	-0.109874	0.241935
23	1	0	5.193093	0.293121	0.222373
24	6	0	3.987910	-1.503512	0.175923
25	1	0	4.843518	-2.169743	0.105162
26	6	0	2.703183	-2.022874	0.202343
27	1	0	2.538976	-3.096574	0.146279
28	6	0	-1.450433	1.017341	-1.741028
29	6	0	-1.654181	-1.252541	-1.755580
30	8	0	-2.355616	-0.051904	-1.681885
31	8	0	-2.213875	-2.311508	-1.863366
32	8	0	-1.832567	2.154801	-1.825629
33	6	0	0.645854	2.543313	0.236516
34	1	0	-0.277668	3.099757	0.444232
35	8	0	1.620752	3.137447	-0.200590

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.457073	0.000000			
3	C	1.423628	2.449914	0.000000		
4	C	2.438448	2.720783	1.441667	0.000000	
5	H	3.414832	3.808321	2.167586	1.089090	0.000000
6	C	3.181199	3.010025	2.775636	2.111305	2.546008
7	H	4.050918	3.718605	3.500243	2.433595	2.570784
8	C	2.867774	2.302066	3.132799	2.890296	3.663541
9	H	3.533155	2.540477	3.984331	3.602442	4.405589
10	C	1.416331	2.550010	2.438467	3.734230	4.597908
11	H	2.179025	2.820329	3.431016	4.613882	5.553587
12	C	2.431479	3.798806	2.793545	4.233471	4.855431
13	H	3.412991	4.684677	3.879927	5.319894	5.926921

This journal is © The Royal Society of Chemistry 2014

14	C	2.825049	4.278266	2.421162	3.759037	4.088719
15	H	3.911307	5.364409	3.408242	4.646238	4.795409
16	C	2.459987	3.757922	1.411220	2.505123	2.712651
17	H	3.438949	4.609872	2.161823	2.737588	2.492326
18	C	2.852438	2.446646	2.467075	1.445054	2.176384
19	C	2.487190	1.456742	2.860673	2.441282	3.420028
20	C	3.770812	2.544131	4.255948	3.737230	4.605519
21	H	4.123983	2.785194	4.897009	4.597595	5.543416
22	C	4.876249	3.793902	5.059012	4.236162	4.864645
23	H	5.837961	4.680370	6.114715	5.322833	5.936343
24	C	5.074354	4.273763	4.853246	3.761695	4.099797
25	H	6.127429	5.360365	5.810687	4.648684	4.806873
26	C	4.243592	3.753344	3.727706	2.505741	2.722361
27	H	4.864552	4.607612	4.056596	2.739394	2.504468
28	C	3.065194	2.985011	3.472261	3.738822	4.446511
29	C	3.568398	3.899817	2.986394	2.810710	2.960904
30	O	3.396477	3.794393	3.296932	3.617458	4.038499
31	O	4.444974	4.953673	3.569249	3.331534	3.080685
32	O	3.627639	3.489131	4.344962	4.803817	5.581775
33	C	2.536954	1.495129	3.804564	4.194070	5.274874
34	H	2.699079	2.209724	4.074165	4.758974	5.815580
35	O	3.675396	2.407073	4.847347	4.990519	6.051563

		6	7	8	9	10
6	C	0.000000				
7	H	1.083122	0.000000			
8	C	1.411935	2.210574	0.000000		
9	H	2.225397	2.655851	1.081258	0.000000	
10	C	4.358212	5.322696	3.902166	4.563050	0.000000
11	H	5.037296	6.009511	4.308765	4.781933	1.084145
12	C	5.022933	5.983186	4.848566	5.664734	1.385672
13	H	6.028701	7.018006	5.757497	6.535797	2.140083
14	C	4.771819	5.621331	5.000724	5.945884	2.430486
15	H	5.652450	6.463757	5.978845	6.959246	3.409606
16	C	3.744801	4.457764	4.260869	5.220500	2.810121
17	H	4.027157	4.549827	4.837317	5.816876	3.896843
18	C	2.687746	2.728167	3.077124	3.366827	4.243791
19	C	3.093053	3.388792	2.794329	2.799051	3.769490
20	C	4.214427	4.296558	3.774369	3.386320	4.909647
21	H	4.867808	5.065215	4.138916	3.594610	5.052618
22	C	4.850545	4.631781	4.710580	4.303938	6.098024
23	H	5.844548	5.585345	5.607303	5.063474	6.989701
24	C	4.605761	4.178532	4.882622	4.690601	6.402064
25	H	5.481526	4.911402	5.859889	5.636418	7.452996
26	C	3.611916	3.227514	4.176832	4.282196	5.613701
27	H	3.921742	3.386935	4.778901	5.015425	6.209728
28	C	2.328230	3.306364	1.480089	2.225438	3.605259
29	C	1.488253	2.217443	2.327904	3.323093	4.405433
30	O	2.332384	3.290334	2.332275	3.308186	3.863771
31	O	2.441145	2.812236	3.503331	4.462960	5.206694
32	O	3.507477	4.451457	2.441601	2.831058	3.796914
33	C	4.057989	4.791523	2.919084	2.782892	2.997869
34	H	4.558121	5.432755	3.390741	3.435106	2.629467

This journal is © The Royal Society of Chemistry 2014

35	O	4.701721	5.256021	3.497737	2.969408	4.202124
		11	12	13	14	15
11	H	0.000000				
12	C	2.132512	0.000000			
13	H	2.443473	1.086514	0.000000		
14	C	3.404083	1.408844	2.164053	0.000000	
15	H	4.290890	2.166330	2.489831	1.086312	0.000000
16	C	3.893875	2.417837	3.398735	1.383912	2.145676
17	H	4.980648	3.409292	4.304154	2.151877	2.483285
18	C	4.902838	5.048482	6.101734	4.848107	5.806962
19	C	4.142572	4.877399	5.836783	5.080306	6.134512
20	C	5.068227	6.103314	6.992099	6.415016	7.468826
21	H	4.977232	6.349533	7.132671	6.874857	7.946671
22	C	6.357205	7.189073	8.124077	7.316813	8.323406
23	H	7.141609	8.127942	9.020819	8.330541	9.342155
24	C	6.874835	7.307228	8.316384	7.161050	8.088815
25	H	7.942447	8.310194	9.323502	8.085817	8.968549
26	C	6.259446	6.360979	7.414118	6.036864	6.918595
27	H	6.969978	6.773369	7.841476	6.228754	6.998143
28	C	3.931278	4.369099	5.115620	4.650957	5.531984
29	C	5.175493	4.715661	5.633880	4.287033	4.986417
30	O	4.457199	4.201616	4.963664	4.111429	4.821999
31	O	6.075036	5.247225	6.132770	4.527636	5.012067
32	O	3.812202	4.604830	5.145563	5.173074	6.019211
33	C	2.700586	4.376367	5.023169	5.208178	6.269176
34	H	2.045316	3.940577	4.403012	4.976313	5.973833
35	O	3.816735	5.585620	6.201690	6.409670	7.477110
		16	17	18	19	20
16	C	0.000000				
17	H	1.086821	0.000000			
18	C	3.729420	4.062544	0.000000		
19	C	4.253653	4.876038	1.421726	0.000000	
20	C	5.630680	6.230358	2.440113	1.414273	0.000000
21	H	6.261221	6.975857	3.420078	2.160076	1.082367
22	C	6.376699	6.795392	2.794060	2.427695	1.387491
23	H	7.433598	7.867734	3.880726	3.410097	2.141866
24	C	6.045530	6.245345	2.421353	2.820632	2.432630
25	H	6.925378	7.014031	3.408371	3.907246	3.412414
26	C	4.828663	4.931814	1.409789	2.455800	2.812686
27	H	4.924878	4.785384	2.162237	3.436680	3.900268
28	C	4.248962	4.911255	4.279953	3.952626	5.009439
29	C	3.419232	3.581048	3.864094	4.325051	5.570328
30	O	3.666072	4.120979	4.571557	4.642594	5.874412
31	O	3.615714	3.429614	4.545639	5.257919	6.519941
32	O	5.049977	5.822032	5.234166	4.653597	5.564391
33	C	4.979175	5.922482	3.824085	2.568253	3.040052
34	H	5.026629	6.045136	4.654662	3.521416	4.115672
35	O	6.103693	6.999051	4.329962	2.954205	2.853388
		21	22	23	24	25
21	H	0.000000				
22	C	2.151571	0.000000			
23	H	2.473786	1.086756	0.000000		

24	C	3.416262	1.408914	2.163912	0.000000	
25	H	4.308811	2.167192	2.490310	1.086709	0.000000
26	C	3.894872	2.419501	3.400572	1.385987	2.147569
27	H	4.982395	3.411109	4.305829	2.153634	2.484275
28	C	5.216423	6.078626	6.965334	6.293249	7.292445
29	C	6.170182	6.275366	7.292910	5.968827	6.820830
30	O	6.260261	6.816975	7.792834	6.767492	7.714034
31	O	7.210960	7.086071	8.123889	6.578275	7.328165
32	O	5.546505	6.752982	7.551164	7.160128	8.185338
33	C	2.710798	4.422440	5.073554	5.248791	6.312728
34	H	3.758514	5.499929	6.152696	6.281500	7.355893
35	O	2.167452	4.160674	4.585926	5.223380	6.216589

		26	27	28	29	30
26	C	0.000000				
27	H	1.087630	0.000000			
28	C	5.502011	6.033374	0.000000		
29	C	4.838750	4.959848	2.279054	0.000000	
30	O	5.746868	6.047250	1.402191	1.392469	0.000000
31	O	5.341153	5.219635	3.417461	1.202616	2.271307
32	O	6.491431	7.111663	1.202913	3.412727	2.272398
33	C	5.008376	5.949822	3.260934	4.864886	4.407293
34	H	5.931723	6.812987	3.238395	5.067195	4.332576
35	O	5.287998	6.310822	4.037323	5.693432	5.308267

		31	32	33	34	35
31	O	0.000000				
32	O	4.482715	0.000000			
33	C	6.013055	3.247454	0.000000		
34	H	6.193197	2.909111	1.098030	0.000000	
35	O	6.867335	3.941035	1.222490	2.005297	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.547772	0.572562	1.129021
2	6	0	0.592306	1.082191	0.378315
3	6	0	-0.732121	-0.839072	1.124449
4	6	0	0.228239	-1.614123	0.379192
5	1	0	0.058528	-2.688009	0.315292
6	6	0	-0.229800	-1.033690	-1.598409
7	1	0	0.462773	-1.739849	-2.039810
8	6	0	-0.103875	0.369167	-1.696880
9	1	0	0.719872	0.901126	-2.152489
10	6	0	-1.500619	1.372532	1.805872
11	1	0	-1.385821	2.449598	1.851905
12	6	0	-2.575758	0.785325	2.453445

```
   13          1               0       -3.284316    1.412215    2.987736
   14          6               0       -2.762329   -0.610795    2.423744
   15          1               0       -3.616682   -1.054584    2.926940
   16          6               0       -1.857218   -1.414365    1.752730
   17          1               0       -1.994326   -2.491840    1.714934
   18          6               0        1.596341   -1.148935    0.370322
   19          6               0        1.793779    0.258886    0.351296
   20          6               0        3.112027    0.758916    0.240111
   21          1               0        3.269867    1.829134    0.204957
   22          6               0        4.186454   -0.117343    0.186188
   23          1               0        5.196641    0.279433    0.130229
   24          6               0        3.984169   -1.511610    0.198002
   25          1               0        4.836125   -2.184559    0.150598
   26          6               0        2.698037   -2.022964    0.271095
   27          1               0        2.528988   -3.097368    0.275190
   28          6               0       -1.472588    0.927459   -1.771699
   29          6               0       -1.685043   -1.338985   -1.661332
   30          8               0       -2.380796   -0.132948   -1.641960
   31          8               0       -2.250246   -2.399655   -1.703875
   32          8               0       -1.851669    2.060468   -1.911663
   33          6               0        0.658587    2.547782    0.090111
   34          1               0       -0.259650    3.118760    0.281148
   35          8               0        1.629098    3.113175   -0.392509
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3926505      0.2605368
0.2438110
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1911.1813755428 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1032.13738670     A.U. after   16 cycles
             Convg  =    0.4953D-08             -V/T =  2.0093
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000713924   -0.000445358    0.000806643
    2          6          -0.000673515    0.002673100    0.002137507
    3          6          -0.000206337    0.000217674   -0.000016033
    4          6           0.000026925    0.000069886   -0.000908978
    5          1          -0.000005372    0.000333974   -0.000229434
```

6	6	0.000228902	-0.000821419	0.001474705
7	1	0.000004429	0.000060849	0.000131899
8	6	-0.000591658	0.000123786	-0.002051651
9	1	0.000124299	0.000366246	0.000100726
10	6	0.000298583	0.000001322	-0.000101657
11	1	-0.000145372	-0.000088600	0.000076480
12	6	-0.000101645	-0.000115356	0.000027826
13	1	0.000023129	0.000005628	0.000015995
14	6	-0.000053649	0.000092517	0.000093568
15	1	-0.000003205	0.000016633	-0.000013824
16	6	0.000128725	-0.000034885	-0.000039778
17	1	0.000001512	0.000013585	-0.000007891
18	6	-0.000029090	-0.000088423	-0.000115240
19	6	0.001156718	-0.000527336	-0.000494247
20	6	0.001052994	0.000006461	0.000650771
21	1	0.001110169	-0.001422517	0.000017808
22	6	-0.000206254	-0.000363810	0.000043571
23	1	-0.000014325	0.000000746	0.000065041
24	6	-0.000011422	0.000060252	-0.000094033
25	1	-0.000016456	-0.000032457	-0.000000030
26	6	0.000055037	-0.000005966	0.000017188
27	1	-0.000011203	0.000004844	0.000023972
28	6	-0.000208193	0.000022581	-0.000069437
29	6	-0.000119608	-0.000043272	-0.000050691
30	8	0.000015347	0.000039060	-0.000054109
31	8	0.000024136	0.000008946	0.000028681
32	8	-0.000040257	-0.000058045	0.000081030
33	6	0.005027377	-0.001344769	-0.003312456
34	1	-0.002107051	0.000849364	0.000262923
35	8	-0.004019746	0.000424759	0.001503154

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.005027377 RMS     0.000932530


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.003049611 RMS     0.000402529
 Search for a saddle point.
 Step number   3 out of a maximum of 202
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Update second derivatives using D2CorX and points  1  2  3
     Eigenvalues ---   -0.01915   0.00159   0.00365   0.00718
0.00854
     Eigenvalues ---    0.01072   0.01255   0.01437   0.01472
0.01523
     Eigenvalues ---    0.01601   0.01706   0.01758   0.01801
0.01913
     Eigenvalues ---    0.01975   0.02111   0.02175   0.02191
0.02233
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02359   0.02427   0.02449   0.02515
0.02686
     Eigenvalues ---    0.02727   0.02746   0.02753   0.03266
0.03539
     Eigenvalues ---    0.04203   0.05548   0.07040   0.07500
0.07841
     Eigenvalues ---    0.08804   0.10209   0.11069   0.11181
0.11226
     Eigenvalues ---    0.11855   0.12291   0.12500   0.12527
0.12662
     Eigenvalues ---    0.12838   0.13915   0.14294   0.14679
0.16393
     Eigenvalues ---    0.17698   0.18525   0.19086   0.19183
0.19336
     Eigenvalues ---    0.19423   0.20130   0.20437   0.20923
0.21173
     Eigenvalues ---    0.23367   0.23906   0.24414   0.25101
0.26083
     Eigenvalues ---    0.27644   0.27938   0.29118   0.30150
0.30353
     Eigenvalues ---    0.31251   0.33098   0.34002   0.34051
0.35022
     Eigenvalues ---    0.35286   0.35920   0.36086   0.36133
0.36203
     Eigenvalues ---    0.36238   0.36330   0.36537   0.37440
0.37835
     Eigenvalues ---    0.38857   0.39872   0.40322   0.41136
0.42461
     Eigenvalues ---    0.44489   0.46449   0.47306   0.47639
0.50257
     Eigenvalues ---    0.50621   0.79400   0.89039
0.902541000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
          1             -0.04485   0.02329   0.17092   0.01790
0.40102
                           R6        R7        R8        R9        R10
          1              0.12718  -0.04518  -0.02026  -0.05880
0.18236
                           R11       R12       R13       R14       R15
          1              0.01904  -0.00793   0.42122   0.16824  -
0.05774
                           R16       R17       R18       R19       R20
          1              0.27237  -0.00769  -0.09477   0.17575  -
0.01032
                           R21       R22       R23       R24       R25
          1             -0.03074  -0.00725   0.17555  -0.00918  -
0.02794
                           R26       R27       R28       R29       R30
          1              0.08113  -0.00133  -0.01375   0.00007
0.01468
                           R31       R32       R33       R34       R35
          1             -0.00022  -0.01587  -0.00027   0.02093
0.01789
                           R36       R37       R38       R39       R40
          1              0.01735  -0.00161  -0.01225  -0.04390
0.00008
                           R41       R42       R43       R44       R45
          1              0.01339  -0.00013  -0.01507  -0.00013
0.00344
                           R46       R47       R48       R49       R50
          1              0.00099  -0.00292   0.00261  -0.00086
0.00538
                           A1        A2        A3        A4        A5
          1              0.02173  -0.00913  -0.01252   0.03584
0.00488
                           A6        A7        A8        A9        A10
```

This journal is © The Royal Society of Chemistry 2014

1	0.01047	0.01851	-0.00183	-0.01590	0.02874

	A11	A12	A13	A14	A15
1	0.05436	0.02491	0.05605	0.03626	0.01820

	A16	A17	A18	A19	A20
1	0.05234	0.01166	0.02275	-0.00419	0.00650

	A21	A22	A23	A24	A25
1	-0.00232	-0.00106	0.00465	-0.00359	-0.00152

	A26	A27	A28	A29	A30
1	-0.00101	0.00253	0.00412	-0.00645	0.00227

	A31	A32	A33	A34	A35
1	0.01942	-0.01771	-0.00085	0.02178	-0.00860

	A36	A37	A38	A39	A40
1	-0.01291	-0.00298	0.00669	-0.00374	-0.00112

	A41	A42	A43	A44	A45
1	0.00437	-0.00324	-0.00117	-0.00141	0.00258

	A46	A47	A48	A49	A50
1	0.00414	-0.00628	0.00204	-0.00395	0.00384

	A51	A52	A53	A54	A55
1	0.00012	-0.00520	0.00233	0.00294	-0.01367

	A56	A57	A58	D1	D2
1	-0.00151	0.00918	-0.00788	0.13778	-0.01355

	D3	D4	D5	D6	D7
1	0.13588	-0.01545	0.01240	0.00096	0.01418

	D8	D9	D10	D11	D12
1	0.00274	0.00118	0.00166	-0.00160	-0.00111

	D13	D14	D15	D16	D17
1	-0.13803	-0.13279	0.01617	0.02141	0.10059

	D18	D19	D20	D21	D22
1	0.10486	-0.06188	-0.05761	0.05198	-0.15521

	D23	D24	D25	D26	D27
1	0.06439	-0.14280	-0.00257	0.00193	-0.01621

	D28	D29	D30	D31	D32
1	-0.01171	0.15476	0.14386	-0.05478	-0.06569

	D33	D34	D35	D36	D37

```
          1              0.00098   0.17379  -0.17469  -0.00188  -
0.14568
                           D38       D39       D40       D41       D42
          1             -0.14998   0.02677   0.02247  -0.02341  -
0.01986
                           D43       D44       D45       D46       D47
          1              0.14775   0.15131  -0.00151  -0.00112  -
0.00100
                           D48       D49       D50       D51       D52
          1             -0.00060  -0.00046   0.00142  -0.00006
0.00182
                           D53       D54       D55       D56       D57
          1              0.00047  -0.00417   0.00236  -0.00228  -
0.01070
                           D58       D59       D60       D61       D62
          1             -0.01567  -0.00106  -0.00603   0.01474
0.00987
                           D63       D64       D65       D66       D67
          1              0.00248  -0.00239   0.00244  -0.00137
0.00887
                           D68       D69       D70       D71       D72
          1              0.00506   0.00211  -0.00026  -0.00175  -
0.00412
                           D73       D74       D75       D76       D77
          1              0.00134  -0.00323  -0.00104  -0.00561
0.00211
                           D78       D79       D80       D81       D82
          1              0.00716  -0.00246   0.00259   0.04275
0.03959
                           D83       D84
          1             -0.04492  -0.04103
 RFO step:  Lambda0=4.322842527D-07 Lambda=-1.16322176D-03.
 Linear search not attempted -- option 19 set.
 Maximum step size (   0.300) exceeded in Quadratic search.
    -- Step size scaled by   0.547
 Iteration  1 RMS(Cart)=  0.02535836 RMS(Int)=  0.00085759
 Iteration  2 RMS(Cart)=  0.00104180 RMS(Int)=  0.00015575
 Iteration  3 RMS(Cart)=  0.00000128 RMS(Int)=  0.00015575
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00015575
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.75347   0.00083   0.00000  -0.00270  -0.00268
2.75079
    R2        2.69027  -0.00004   0.00000  -0.00075  -0.00069
2.68958
    R3        5.41931   0.00043   0.00000   0.05116   0.05121
5.47051
    R4        2.67648  -0.00005   0.00000   0.00046   0.00046
2.67694
    R5        4.35027   0.00071   0.00000   0.09975   0.09988
4.45015
```

This journal is © The Royal Society of Chemistry 2014

R6	4.80081	-0.00001	0.00000	0.06651	0.06666
4.86746					
R7	2.75284	0.00117	0.00000	-0.00180	-0.00229
2.75056					
R8	2.82538	-0.00110	0.00000	-0.00546	-0.00564
2.81975					
R9	2.72436	0.00019	0.00000	0.00321	0.00325
2.72760					
R10	5.24519	-0.00007	0.00000	-0.02885	-0.02889
5.21631					
R11	2.66682	-0.00005	0.00000	-0.00103	-0.00103
2.66579					
R12	2.05808	0.00001	0.00000	-0.00020	-0.00017
2.05792					
R13	3.98979	-0.00042	0.00000	-0.06751	-0.06755
3.92224					
R14	4.59883	-0.00017	0.00000	-0.04845	-0.04846
4.55037					
R15	2.73076	0.00003	0.00000	0.00346	0.00355
2.73431					
R16	4.81126	-0.00054	0.00000	-0.07207	-0.07213
4.73913					
R17	2.04680	0.00006	0.00000	0.00068	0.00067
2.04748					
R18	2.66817	0.00034	0.00000	0.00037	0.00035
2.66852					
R19	5.07910	-0.00007	0.00000	-0.02502	-0.02495
5.05416					
R20	2.81239	0.00006	0.00000	0.00643	0.00644
2.81883					
R21	5.15549	-0.00027	0.00000	-0.01210	-0.01207
5.14342					
R22	2.04328	0.00020	0.00000	-0.00061	-0.00066
2.04263					
R23	5.28052	0.00083	0.00000	0.06128	0.06116
5.34168					
R24	2.79696	0.00025	0.00000	-0.00630	-0.00629
2.79067					
R25	5.28944	0.00035	0.00000	0.03700	0.03699
5.32643					
R26	5.25890	-0.00034	0.00000	0.03788	0.03768
5.29659					
R27	2.04874	-0.00010	0.00000	0.00027	0.00027
2.04901					
R28	2.61854	0.00010	0.00000	-0.00019	-0.00019
2.61835					
R29	2.05321	-0.00001	0.00000	-0.00001	-0.00001
2.05321					
R30	2.66233	-0.00013	0.00000	0.00019	0.00019
2.66252					
R31	2.05283	-0.00001	0.00000	0.00000	0.00000
2.05283					

This journal is © The Royal Society of Chemistry 2014

R32	2.61521	0.00003	0.00000	0.00068	0.00068
2.61589					
R33	2.05379	-0.00001	0.00000	-0.00007	-0.00007
2.05372					
R34	2.68667	0.00009	0.00000	0.00113	0.00100
2.68768					
R35	2.66412	-0.00001	0.00000	-0.00113	-0.00113
2.66299					
R36	2.67259	0.00020	0.00000	0.00171	0.00138
2.67397					
R37	2.04538	-0.00016	0.00000	-0.00084	-0.00063
2.04474					
R38	2.62198	0.00005	0.00000	-0.00007	-0.00008
2.62190					
R39	4.09589	0.00224	0.00000	0.04556	0.04599
4.14188					
R40	2.05367	-0.00001	0.00000	0.00002	0.00002
2.05369					
R41	2.66246	-0.00012	0.00000	-0.00042	-0.00030
2.66216					
R42	2.05358	0.00001	0.00000	0.00001	0.00001
2.05359					
R43	2.61914	-0.00013	0.00000	0.00029	0.00042
2.61956					
R44	2.05532	-0.00001	0.00000	0.00004	0.00004
2.05536					
R45	2.64976	-0.00001	0.00000	0.00513	0.00510
2.65486					
R46	2.27318	-0.00005	0.00000	0.00020	0.00020
2.27338					
R47	2.63139	-0.00001	0.00000	-0.00543	-0.00547
2.62592					
R48	2.27262	-0.00002	0.00000	-0.00018	-0.00018
2.27243					
R49	2.07498	0.00226	0.00000	0.00483	0.00483
2.07980					
R50	2.31017	-0.00305	0.00000	-0.00146	-0.00137
2.30880					
A1	2.03363	-0.00005	0.00000	0.00318	0.00317
2.03680					
A2	2.18347	0.00014	0.00000	-0.00384	-0.00388
2.17959					
A3	2.06517	-0.00009	0.00000	0.00117	0.00115
2.06632					
A4	2.04566	-0.00017	0.00000	0.00293	0.00283
2.04849					
A5	2.06787	0.00033	0.00000	-0.00232	-0.00213
2.06574					
A6	2.11048	-0.00007	0.00000	0.01428	0.01318
2.12366					
A7	2.03586	0.00017	0.00000	-0.00168	-0.00170
2.03416					

This journal is © The Royal Society of Chemistry 2014

A8	2.10137	0.00005	0.00000	-0.00034	-0.00034
2.10103					
A9	2.14370	-0.00022	0.00000	0.00188	0.00190
2.14559					
A10	2.04500	-0.00010	0.00000	-0.00290	-0.00297
2.04203					
A11	2.04967	0.00014	0.00000	-0.00479	-0.00491
2.04476					
A12	2.05397	-0.00010	0.00000	-0.00361	-0.00367
2.05030					
A13	2.16799	-0.00005	0.00000	-0.00689	-0.00708
2.16092					
A14	2.06493	-0.00009	0.00000	-0.00527	-0.00544
2.05949					
A15	1.86301	0.00005	0.00000	-0.00475	-0.00478
1.85823					
A16	2.19710	0.00007	0.00000	0.00726	0.00689
2.20399					
A17	1.87112	-0.00018	0.00000	0.00436	0.00430
1.87541					
A18	2.09167	0.00015	0.00000	0.00597	0.00574
2.09741					
A19	2.10620	0.00015	0.00000	-0.00110	-0.00110
2.10509					
A20	2.10130	0.00004	0.00000	-0.00076	-0.00076
2.10055					
A21	2.07524	-0.00019	0.00000	0.00175	0.00174
2.07698					
A22	2.08438	-0.00002	0.00000	0.00039	0.00038
2.08476					
A23	2.10929	0.00002	0.00000	-0.00033	-0.00033
2.10896					
A24	2.08951	0.00000	0.00000	-0.00005	-0.00005
2.08946					
A25	2.09350	0.00002	0.00000	-0.00025	-0.00025
2.09325					
A26	2.09326	-0.00006	0.00000	0.00055	0.00056
2.09382					
A27	2.09642	0.00004	0.00000	-0.00030	-0.00031
2.09612					
A28	2.09507	0.00003	0.00000	-0.00023	-0.00023
2.09483					
A29	2.08202	-0.00002	0.00000	0.00042	0.00042
2.08244					
A30	2.10599	-0.00001	0.00000	-0.00019	-0.00019
2.10581					
A31	2.03793	0.00010	0.00000	0.00099	0.00091
2.03884					
A32	2.14206	-0.00021	0.00000	-0.00199	-0.00173
2.14033					
A33	2.09953	0.00011	0.00000	0.00082	0.00064
2.10017					

A34	2.03181	-0.00007	0.00000	-0.00057	-0.00033	2.03148
A35	2.17780	0.00028	0.00000	0.00209	0.00146	2.17926
A36	2.07213	-0.00021	0.00000	-0.00108	-0.00073	2.07140
A37	2.08067	-0.00055	0.00000	0.00155	0.00124	2.08192
A38	2.09619	0.00001	0.00000	-0.00036	-0.00045	2.09574
A39	2.10629	0.00055	0.00000	-0.00122	-0.00081	2.10548
A40	2.08430	-0.00006	0.00000	-0.00079	-0.00074	2.08356
A41	2.11002	0.00009	0.00000	0.00093	0.00084	2.11086
A42	2.08886	-0.00003	0.00000	-0.00013	-0.00009	2.08876
A43	2.09427	0.00005	0.00000	0.00032	0.00029	2.09456
A44	2.09299	-0.00004	0.00000	-0.00044	-0.00038	2.09261
A45	2.09593	-0.00001	0.00000	0.00013	0.00010	2.09602
A46	2.09455	0.00004	0.00000	0.00014	0.00009	2.09464
A47	2.08370	-0.00003	0.00000	-0.00006	-0.00003	2.08366
A48	2.10469	-0.00001	0.00000	-0.00010	-0.00007	2.10462
A49	1.88497	0.00006	0.00000	-0.00121	-0.00119	1.88378
A50	2.28179	0.00004	0.00000	0.00381	0.00380	2.28558
A51	2.11642	-0.00010	0.00000	-0.00259	-0.00260	2.11382
A52	1.88632	0.00000	0.00000	0.00088	0.00089	1.88720
A53	2.26787	-0.00002	0.00000	-0.00374	-0.00374	2.26412
A54	2.12887	0.00003	0.00000	0.00282	0.00282	2.13169
A55	1.90719	0.00007	0.00000	0.00022	0.00017	1.90736
A56	2.02541	-0.00080	0.00000	-0.01205	-0.01175	2.01367
A57	2.17080	0.00100	0.00000	0.01080	0.01020	2.18101
A58	2.08527	-0.00016	0.00000	0.00104	0.00134	2.08661
D1	-0.59775	0.00023	0.00000	0.01194	0.01200	-0.58575

This journal is © The Royal Society of Chemistry 2014

D2	2.90286	-0.00001	0.00000	-0.03446	-0.03388	2.86898
D3	2.59089	0.00016	0.00000	-0.00115	-0.00119	2.58969
D4	-0.19169	-0.00008	0.00000	-0.04755	-0.04707	-0.23876
D5	0.00078	0.00004	0.00000	-0.01418	-0.01417	-0.01338
D6	-3.07063	-0.00004	0.00000	-0.01207	-0.01213	-3.08277
D7	3.09866	0.00011	0.00000	-0.00216	-0.00201	3.09665
D8	0.02724	0.00003	0.00000	-0.00005	0.00002	0.02726
D9	-0.07132	0.00004	0.00000	0.00797	0.00802	-0.06330
D10	3.10275	0.00004	0.00000	0.01202	0.01204	3.11479
D11	3.11809	-0.00003	0.00000	-0.00539	-0.00543	3.11266
D12	0.00897	-0.00003	0.00000	-0.00133	-0.00141	0.00757
D13	0.58219	-0.00032	0.00000	-0.00941	-0.00945	0.57274
D14	-2.61818	-0.00020	0.00000	-0.00066	-0.00075	-2.61893
D15	-2.92766	0.00001	0.00000	0.03451	0.03464	-2.89303
D16	0.15515	0.00013	0.00000	0.04326	0.04333	0.19848
D17	-0.21524	-0.00011	0.00000	-0.07075	-0.07078	-0.28601
D18	2.98947	-0.00086	0.00000	-0.06686	-0.06701	2.92246
D19	-2.98401	-0.00035	0.00000	-0.11635	-0.11634	-3.10034
D20	0.22070	-0.00109	0.00000	-0.11247	-0.11257	0.10812
D21	-3.07321	-0.00012	0.00000	-0.01075	-0.01081	-3.08402
D22	0.61386	0.00002	0.00000	0.01125	0.01114	0.62500
D23	-0.00365	-0.00003	0.00000	-0.01302	-0.01300	-0.01666
D24	-2.59977	0.00011	0.00000	0.00898	0.00894	-2.59082
D25	-0.04444	-0.00001	0.00000	0.00088	0.00086	-0.04357
D26	3.11258	0.00001	0.00000	0.00077	0.00078	3.11336
D27	-3.11138	-0.00011	0.00000	0.00329	0.00319	-3.10819

This journal is © The Royal Society of Chemistry 2014

D28	0.04564	-0.00008	0.00000	0.00318	0.00310	0.04874
D29	-0.62974	-0.00009	0.00000	-0.00842	-0.00837	-0.63812
D30	2.60355	-0.00008	0.00000	-0.00632	-0.00623	2.59732
D31	3.06016	0.00005	0.00000	0.01347	0.01346	3.07362
D32	0.01028	0.00007	0.00000	0.01557	0.01560	0.02588
D33	-0.08214	-0.00021	0.00000	-0.04869	-0.04868	-0.13082
D34	2.53788	-0.00009	0.00000	-0.01293	-0.01284	2.52505
D35	-2.58609	-0.00006	0.00000	-0.02168	-0.02176	-2.60786
D36	0.03393	0.00005	0.00000	0.01408	0.01407	0.04801
D37	-2.66243	0.00009	0.00000	0.01407	0.01404	-2.64838
D38	0.49688	0.00009	0.00000	0.01633	0.01630	0.51318
D39	-0.11419	-0.00004	0.00000	-0.01176	-0.01174	-0.12593
D40	3.04512	-0.00004	0.00000	-0.00951	-0.00948	3.03563
D41	0.05665	-0.00005	0.00000	-0.01225	-0.01227	0.04438
D42	-3.08867	-0.00009	0.00000	-0.00813	-0.00813	-3.09680
D43	2.71416	0.00004	0.00000	0.02143	0.02140	2.73557
D44	-0.43115	0.00000	0.00000	0.02555	0.02554	-0.40561
D45	3.11636	0.00000	0.00000	-0.00042	-0.00040	3.11596
D46	-0.02856	0.00001	0.00000	0.00193	0.00196	-0.02660
D47	0.00667	-0.00001	0.00000	0.00361	0.00361	0.01028
D48	-3.13825	0.00001	0.00000	0.00597	0.00597	-3.13228
D49	-3.12933	-0.00001	0.00000	-0.00160	-0.00161	-3.13094
D50	0.01151	0.00001	0.00000	-0.00108	-0.00106	0.01045
D51	0.00893	0.00001	0.00000	0.00076	0.00075	0.00968
D52	-3.13341	0.00003	0.00000	0.00128	0.00130	-3.13211
D53	0.02498	-0.00001	0.00000	-0.00031	-0.00034	0.02464

This journal is © The Royal Society of Chemistry 2014

D54	-3.13226	-0.00004	0.00000	-0.00020	-0.00025	-3.13251
D55	-3.11737	0.00000	0.00000	0.00021	0.00021	-3.11715
D56	0.00858	-0.00002	0.00000	0.00033	0.00031	0.00889
D57	0.02724	0.00018	0.00000	0.00814	0.00815	0.03539
D58	-3.05930	0.00005	0.00000	-0.00017	-0.00006	-3.05936
D59	3.07949	0.00015	0.00000	0.00593	0.00593	3.08542
D60	-0.00705	0.00002	0.00000	-0.00237	-0.00229	-0.00933
D61	3.08324	-0.00001	0.00000	-0.00072	-0.00080	3.08245
D62	-0.08213	-0.00002	0.00000	-0.00140	-0.00145	-0.08358
D63	0.03649	0.00000	0.00000	0.00145	0.00141	0.03790
D64	-3.12889	-0.00001	0.00000	0.00077	0.00076	-3.12813
D65	0.03889	-0.00037	0.00000	-0.00409	-0.00414	0.03475
D66	-3.11013	-0.00015	0.00000	-0.00686	-0.00687	-3.11700
D67	3.12045	-0.00024	0.00000	0.00486	0.00476	3.12521
D68	-0.02857	-0.00002	0.00000	0.00210	0.00202	-0.02655
D69	-3.11038	-0.00002	0.00000	0.00086	0.00086	-3.10952
D70	0.03539	0.00001	0.00000	-0.00088	-0.00087	0.03452
D71	0.02367	0.00020	0.00000	-0.00194	-0.00190	0.02177
D72	-3.11374	0.00023	0.00000	-0.00367	-0.00363	-3.11737
D73	3.13669	-0.00001	0.00000	0.00085	0.00085	3.13754
D74	-0.00572	0.00000	0.00000	-0.00009	-0.00006	-0.00578
D75	-0.00072	0.00003	0.00000	-0.00089	-0.00089	-0.00160
D76	3.14006	0.00004	0.00000	-0.00183	-0.00179	3.13827
D77	-0.03021	-0.00001	0.00000	-0.00020	-0.00022	-0.03043
D78	3.13546	0.00000	0.00000	0.00049	0.00044	3.13590
D79	3.11057	0.00000	0.00000	-0.00115	-0.00113	3.10944

```
   D80       -0.00696   0.00001   0.00000  -0.00045  -0.00047  -
0.00742
   D81       -0.13099   0.00002   0.00000   0.00467   0.00466  -
0.12633
   D82        3.01390   0.00005   0.00000   0.00100   0.00099
3.01490
   D83        0.15212   0.00001   0.00000   0.00420   0.00421
0.15633
   D84       -3.00549   0.00001   0.00000   0.00209   0.00209  -
3.00340
         Item               Value     Threshold  Converged?
 Maximum Force            0.003050     0.000450     NO
 RMS     Force            0.000403     0.000300     NO
 Maximum Displacement     0.175984     0.001800     NO
 RMS     Displacement     0.025297     0.001200     NO
 Predicted change in Energy=-5.143978D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.560903    0.517637    1.155620
    2          6             0        0.593203    1.075646    0.465990
    3          6             0       -0.743797   -0.890581    1.059933
    4          6             0        0.226087   -1.615171    0.274021
    5          1             0        0.062395   -2.684637    0.150042
    6          6             0       -0.203517   -0.954941   -1.646261
    7          1             0        0.495088   -1.635093   -2.118776
    8          6             0       -0.089100    0.451516   -1.699781
    9          1             0        0.742708    1.010615   -2.104595
   10          6             0       -1.521026    1.274482    1.871189
   11          1             0       -1.403064    2.345835    1.989396
   12          6             0       -2.603458    0.647969    2.467536
   13          1             0       -3.318075    1.239583    3.033062
   14          6             0       -2.788089   -0.743723    2.348239
   15          1             0       -3.647351   -1.218404    2.813447
   16          6             0       -1.874726   -1.504063    1.638414
   17          1             0       -2.010713   -2.577062    1.532220
   18          6             0        1.595583   -1.150740    0.323025
   19          6             0        1.793865    0.255560    0.399326
   20          6             0        3.115298    0.758904    0.347349
   21          1             0        3.276458    1.828049    0.389171
   22          6             0        4.189133   -0.114911    0.256038
   23          1             0        5.200600    0.282476    0.247152
   24          6             0        3.985648   -1.506356    0.171988
   25          1             0        4.837691   -2.176711    0.097206
   26          6             0        2.697579   -2.018443    0.186920
   27          1             0        2.527365   -3.090433    0.117326
```

28	6	0	-1.456709	1.005051	-1.763569
29	6	0	-1.659171	-1.264917	-1.746465
30	8	0	-2.361304	-0.067202	-1.688111
31	8	0	-2.213903	-2.327653	-1.840903
32	8	0	-1.844357	2.139643	-1.861995
33	6	0	0.637053	2.549270	0.235759
34	1	0	-0.323788	3.073449	0.351106
35	8	0	1.623759	3.172286	-0.126148

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.455653	0.000000			
3	C	1.423265	2.450793	0.000000		
4	C	2.438327	2.722521	1.443386	0.000000	
5	H	3.413832	3.810684	2.167138	1.089002	0.000000
6	C	3.185396	3.036388	2.760350	2.075559	2.507840
7	H	4.058452	3.746833	3.491895	2.407953	2.536986
8	C	2.894872	2.354919	3.137813	2.875139	3.644208
9	H	3.545621	2.575750	3.979758	3.580427	4.381906
10	C	1.416577	2.546387	2.439204	3.735431	4.598282
11	H	2.178699	2.814112	3.431169	4.613698	5.553058
12	C	2.431078	3.795752	2.794069	4.235521	4.856318
13	H	3.412915	4.681328	3.880430	5.321936	5.927806
14	C	2.823779	4.276225	2.420832	3.761258	4.089558
15	H	3.910037	5.362418	3.407771	4.648616	4.796435
16	C	2.458961	3.757679	1.410673	2.507454	2.713199
17	H	3.438159	4.610803	2.161562	2.740725	2.493946
18	C	2.850812	2.445813	2.466458	1.446934	2.175644
19	C	2.487087	1.455533	2.861778	2.444026	3.421241
20	C	3.771733	2.544673	4.256899	3.740207	4.606205
21	H	4.126738	2.787807	4.899319	4.601499	5.545424
22	C	4.875676	3.793708	5.057837	4.237551	4.862582
23	H	5.837426	4.680290	6.113308	5.324243	5.934167
24	C	5.072988	4.273389	4.851317	3.762519	4.096430
25	H	6.125730	5.359991	5.808096	4.649030	4.802523
26	C	4.241201	3.752288	3.725224	2.505692	2.718340
27	H	4.861443	4.606383	4.053192	2.738035	2.498363
28	C	3.092200	3.029531	3.474741	3.721442	4.425312
29	C	3.578517	3.930189	2.975551	2.785541	2.928504
30	O	3.416179	3.830844	3.293331	3.597327	4.012991
31	O	4.450531	4.978358	3.555452	3.306672	3.045132
32	O	3.658437	3.534587	4.350994	4.790400	5.563963
33	C	2.531556	1.492145	3.797181	4.184844	5.266058
34	H	2.689915	2.201202	4.048750	4.721383	5.774524
35	O	3.669174	2.410097	4.849638	5.003335	6.067758

		6	7	8	9	10
6	C	0.000000				
7	H	1.083479	0.000000			
8	C	1.412118	2.206982	0.000000		
9	H	2.229085	2.657308	1.080912	0.000000	
10	C	4.367907	5.333870	3.934401	4.582682	0.000000

This journal is © The Royal Society of Chemistry 2014

11	H	5.054903	6.027259	4.350285	4.811228	1.084290
12	C	5.025173	5.987288	4.871049	5.677386	1.385571
13	H	6.034275	7.024629	5.783349	6.552702	2.140222
14	C	4.762421	5.614982	5.009950	5.947433	2.430263
15	H	5.640780	6.454476	5.984898	6.959043	3.409339
16	C	3.726065	4.444059	4.261020	5.213892	2.810623
17	H	3.999997	4.527264	4.828116	5.803376	3.897318
18	C	2.674544	2.721779	3.081741	3.360385	4.241671
19	C	3.104718	3.406205	2.826695	2.818627	3.767372
20	C	4.233943	4.321863	3.814891	3.421194	4.907485
21	H	4.898801	5.100900	4.193512	3.647870	5.051600
22	C	4.860018	4.647222	4.738074	4.326343	6.094673
23	H	5.858387	5.605046	5.639153	5.092514	6.985831
24	C	4.599912	4.177103	4.892888	4.694106	6.398735
25	H	5.472310	4.905317	5.866004	5.637008	7.449230
26	C	3.592764	3.211567	4.174436	4.271739	5.610414
27	H	3.889510	3.353852	4.763735	4.994049	6.206287
28	C	2.329339	3.302430	1.476762	2.225705	3.645297
29	C	1.491661	2.217313	2.326681	3.327961	4.422110
30	O	2.333641	3.286751	2.330690	3.312105	3.895484
31	O	2.442105	2.809890	3.501212	4.467115	5.218724
32	O	3.509323	4.448322	2.440700	2.833101	3.845739
33	C	4.065471	4.803424	2.945197	2.802833	2.992828
34	H	4.497985	5.379707	3.337027	3.379817	2.642028
35	O	4.762739	5.324975	3.579496	3.059955	4.180991

		11	12	13	14	15
11	H	0.000000				
12	C	2.133615	0.000000			
13	H	2.445465	1.086510	0.000000		
14	C	3.404766	1.408946	2.164109	0.000000	
15	H	4.291817	2.166268	2.489649	1.086311	0.000000
16	C	3.894530	2.418623	3.399395	1.384269	2.145811
17	H	4.981282	3.409837	4.304474	2.152053	2.483159
18	C	4.898440	5.046408	6.099343	4.846002	5.804751
19	C	4.137382	4.875237	5.834107	5.078497	6.132486
20	C	5.062634	6.100137	6.988018	6.411819	7.464905
21	H	4.972600	6.347094	7.129118	6.872459	7.943370
22	C	6.350785	7.184150	8.118170	7.311248	8.316762
23	H	7.134511	8.122008	9.013610	8.323870	9.334064
24	C	6.868811	7.302532	8.310854	7.155501	8.082258
25	H	7.936046	8.304696	9.317018	8.079179	8.960594
26	C	6.253888	6.357040	7.409679	6.032310	6.913526
27	H	6.964620	6.769379	7.837074	6.223992	6.992902
28	C	3.985640	4.398271	5.150471	4.662376	5.540013
29	C	5.201902	4.723200	5.645207	4.279334	4.974718
30	O	4.501670	4.223684	4.991249	4.114844	4.821121
31	O	6.096732	5.250593	6.140024	4.515244	4.994815
32	O	3.882071	4.641785	5.190717	5.189461	6.032167
33	C	2.697908	4.369975	5.018289	5.199805	6.260668
34	H	2.092428	3.944506	4.418338	4.963076	5.960638
35	O	3.784204	5.564955	6.175570	6.397040	7.463509

		16	17	18	19	20

This journal is © The Royal Society of Chemistry 2014

16	C	0.000000				
17	H	1.086783	0.000000			
18	C	3.728019	4.062255	0.000000		
19	C	4.253254	4.876680	1.422258	0.000000	
20	C	5.629228	6.229653	2.440669	1.415006	0.000000
21	H	6.260852	6.976084	3.420951	2.161228	1.082032
22	C	6.372683	6.791828	2.793552	2.427980	1.387449
23	H	7.428834	7.863294	3.880208	3.410238	2.141380
24	C	6.041059	6.241232	2.421092	2.821337	2.433036
25	H	6.919849	7.008579	3.408060	3.907952	3.412777
26	C	4.824665	4.928479	1.409194	2.456197	2.813162
27	H	4.920232	4.781174	2.161698	3.437036	3.900766
28	C	4.247808	4.899049	4.279930	3.975686	5.041806
29	C	3.400156	3.548955	3.858659	4.340475	5.592446
30	O	3.656103	4.097907	4.568991	4.661223	5.900739
31	O	3.591516	3.388429	4.536507	5.268190	6.535722
32	O	5.052759	5.813405	5.237759	4.679744	5.602304
33	C	4.970511	5.913608	3.823149	2.574116	3.059340
34	H	5.001618	6.014069	4.639887	3.525235	4.145412
35	O	6.100927	7.001040	4.346390	2.968560	2.876334

		21	22	23	24	25
21	H	0.000000				
22	C	2.150766	0.000000			
23	H	2.472102	1.086766	0.000000		
24	C	3.415901	1.408755	2.163719	0.000000	
25	H	4.308224	2.167227	2.490339	1.086713	0.000000
26	C	3.895062	2.419286	3.400436	1.386209	2.147830
27	H	4.982621	3.410931	4.305759	2.153805	2.484532
28	C	5.264455	6.099890	6.991772	6.298635	7.294214
29	C	6.203855	6.287702	7.309267	5.966803	6.814668
30	O	6.300114	6.833025	7.813444	6.768673	7.711220
31	O	7.237897	7.091704	8.133118	6.569680	7.314645
32	O	5.602462	6.780272	7.584786	7.170729	8.192627
33	C	2.740466	4.440219	5.095532	5.259778	6.324512
34	H	3.809756	5.526404	6.190250	6.291100	7.366784
35	O	2.191789	4.187228	4.613475	5.249486	6.244279

		26	27	28	29	30
26	C	0.000000				
27	H	1.087649	0.000000			
28	C	5.495820	6.015281	0.000000		
29	C	4.825666	4.932881	2.279043	0.000000	
30	O	5.737193	6.024834	1.404889	1.389575	0.000000
31	O	5.322625	5.186147	3.418515	1.202520	2.270399
32	O	6.489755	7.098124	1.203020	3.411550	2.273243
33	C	5.011203	5.949249	3.281121	4.873384	4.420107
34	H	5.923089	6.795379	3.167590	5.000447	4.263046
35	O	5.309874	6.332254	4.106986	5.752549	5.367936

		31	32	33	34	35
31	O	0.000000				
32	O	4.482605	0.000000			
33	C	6.018708	3.275020	0.000000		
34	H	6.127752	2.842875	1.100583	0.000000	

This journal is © The Royal Society of Chemistry 2014

35 O 6.922237 4.013395 1.221766 2.007605 0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.532771	0.627555	1.110021
2	6	0	0.610765	1.106519	0.347234
3	6	0	-0.728592	-0.781548	1.152041
4	6	0	0.218759	-1.586682	0.418795
5	1	0	0.044169	-2.661436	0.400144
6	6	0	-0.246295	-1.106998	-1.546293
7	1	0	0.436832	-1.835593	-1.966309
8	6	0	-0.122109	0.286899	-1.735254
9	1	0	0.705254	0.797043	-2.208110
10	6	0	-1.471603	1.458046	1.769998
11	1	0	-1.342839	2.534577	1.783657
12	6	0	-2.545992	0.901363	2.444978
13	1	0	-3.243845	1.550779	2.966288
14	6	0	-2.743922	-0.493507	2.461967
15	1	0	-3.596796	-0.913634	2.987487
16	6	0	-1.851743	-1.326478	1.808991
17	1	0	-1.998286	-2.403335	1.807812
18	6	0	1.592555	-1.133068	0.395649
19	6	0	1.803334	0.272142	0.334203
20	6	0	3.127241	0.755406	0.207840
21	1	0	3.297557	1.822089	0.144804
22	6	0	4.192076	-0.133552	0.177956
23	1	0	5.206186	0.251334	0.110837
24	6	0	3.976046	-1.524657	0.230386
25	1	0	4.821077	-2.207352	0.202175
26	6	0	2.684642	-2.020454	0.320029
27	1	0	2.504664	-3.092510	0.355877
28	6	0	-1.486419	0.845214	-1.823387
29	6	0	-1.706111	-1.410865	-1.586996
30	8	0	-2.397520	-0.206218	-1.628194
31	8	0	-2.270964	-2.472312	-1.568923
32	8	0	-1.867235	1.969122	-2.021043
33	6	0	0.661179	2.551241	-0.022539
34	1	0	-0.292899	3.093323	0.062122
35	8	0	1.644807	3.127564	-0.461903

Rotational constants (GHZ): 0.3907477 0.2599865 0.2431988
Standard basis: 6-31+G(d) (6D, 7F)
There are 461 symmetry adapted basis functions of A symmetry.

```
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1909.2317541391 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1032.13786248     A.U. after   16 cycles
             Convg  =    0.3779D-08             -V/T =  2.0093
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000506596   -0.000321468    0.000620355
    2          6          -0.000760429    0.001065526    0.000968774
    3          6          -0.000180443    0.000208686    0.000170912
    4          6          -0.000031918   -0.000179490   -0.000777727
    5          1           0.000026914    0.000177775    0.000000516
    6          6           0.000211344   -0.000728665    0.000916878
    7          1          -0.000012284    0.000027917   -0.000009452
    8          6          -0.000332454    0.000490451   -0.000843836
    9          1           0.000112809    0.000261385   -0.000086621
   10          6           0.000257258    0.000014606   -0.000173719
   11          1          -0.000015092    0.000053664   -0.000026244
   12          6          -0.000092543   -0.000103507    0.000007266
   13          1           0.000010508    0.000004937    0.000005966
   14          6          -0.000040783    0.000118619    0.000093342
   15          1          -0.000000564    0.000014876   -0.000003029
   16          6           0.000164710   -0.000011927   -0.000075547
   17          1           0.000001533    0.000016653   -0.000023307
   18          6           0.000044306   -0.000118717   -0.000067455
   19          6           0.000766770   -0.000437079   -0.000074310
   20          6           0.000687773    0.000010374    0.000297584
   21          1           0.000688615   -0.000841014   -0.000031336
   22          6          -0.000075642   -0.000192342   -0.000018008
   23          1          -0.000002242   -0.000021440    0.000023404
   24          6          -0.000055938    0.000083897   -0.000028375
   25          1          -0.000011757   -0.000014550    0.000002762
   26          6           0.000063583    0.000073858   -0.000006283
   27          1           0.000002337    0.000002435    0.000005682
   28          6          -0.000025742   -0.000055372   -0.000160354
   29          6           0.000013484   -0.000023102   -0.000047600
   30          8          -0.000049017    0.000073141   -0.000047040
   31          8          -0.000042485   -0.000091288    0.000052617
   32          8          -0.000050120    0.000116282    0.000079451
   33          6           0.002541934   -0.000293621   -0.001812905
```

```
   34          1          -0.001140376    0.000415227    0.000170918
   35          8          -0.002167456    0.000203272    0.000896724
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.002541934 RMS     0.000502295


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.001613723 RMS     0.000227849
 Search for a saddle point.
 Step number   4 out of a maximum of 202
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Update second derivatives using D2CorX and points  2  3  4
     Eigenvalues ---   -0.01914   0.00238   0.00370   0.00723
0.00858
     Eigenvalues ---    0.01076   0.01256   0.01437   0.01471
0.01524
     Eigenvalues ---    0.01601   0.01705   0.01760   0.01801
0.01913
     Eigenvalues ---    0.01974   0.02111   0.02174   0.02191
0.02232
     Eigenvalues ---    0.02359   0.02426   0.02449   0.02515
0.02686
     Eigenvalues ---    0.02727   0.02746   0.02753   0.03261
0.03538
     Eigenvalues ---    0.04200   0.05547   0.07036   0.07488
0.07826
     Eigenvalues ---    0.08797   0.10202   0.11060   0.11180
0.11225
     Eigenvalues ---    0.11854   0.12291   0.12499   0.12527
0.12661
     Eigenvalues ---    0.12837   0.13912   0.14288   0.14673
0.16382
     Eigenvalues ---    0.17678   0.18515   0.19087   0.19179
0.19335
     Eigenvalues ---    0.19421   0.20120   0.20430   0.20914
0.21168
     Eigenvalues ---    0.23359   0.23906   0.24408   0.25101
0.26068
     Eigenvalues ---    0.27645   0.27940   0.29115   0.30149
0.30335
     Eigenvalues ---    0.31247   0.33095   0.34000   0.34050
0.35023
     Eigenvalues ---    0.35283   0.35920   0.36086   0.36133
0.36203
     Eigenvalues ---    0.36238   0.36329   0.36536   0.37440
0.37830
     Eigenvalues ---    0.38856   0.39871   0.40321   0.41126
0.42460
```

```
     Eigenvalues ---    0.44488   0.46427   0.47305   0.47638
0.50257
     Eigenvalues ---    0.50620   0.79401   0.89039
0.902561000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
         1             -0.04401   0.02336   0.16535   0.01786
0.39024
                           R6        R7        R8        R9        R10
         1              0.12008  -0.04445  -0.02003  -0.05952
0.18578
                           R11       R12       R13       R14       R15
         1              0.01913  -0.00751   0.42878   0.17308  -
0.05823
                           R16       R17       R18       R19       R20
```

This journal is © The Royal Society of Chemistry 2014

1	0.27887	-0.00757	-0.09468	0.17875	-0.01136

	R21	R22	R23	R24	R25
1	-0.03035	-0.00724	0.16936	-0.00805	-0.03084

	R26	R27	R28	R29	R30
1	0.07754	-0.00138	-0.01372	0.00007	0.01460

	R31	R32	R33	R34	R35
1	-0.00022	-0.01594	-0.00027	0.02094	0.01799

	R36	R37	R38	R39	R40
1	0.01735	-0.00163	-0.01224	-0.04631	0.00008

	R41	R42	R43	R44	R45
1	0.01333	-0.00013	-0.01518	-0.00014	0.00309

	R46	R47	R48	R49	R50
1	0.00096	-0.00265	0.00262	-0.00097	0.00525

	A1	A2	A3	A4	A5
1	0.02176	-0.00898	-0.01276	0.03433	0.00225

	A6	A7	A8	A9	A10
1	0.00680	0.01873	-0.00174	-0.01616	0.03097

	A11	A12	A13	A14	A15
1	0.05549	0.02725	0.05848	0.03882	0.02013

	A16	A17	A18	A19	A20
1	0.04972	0.00965	0.01948	-0.00402	0.00664

	A21	A22	A23	A24	A25
1	-0.00261	-0.00112	0.00470	-0.00358	-0.00147

	A26	A27	A28	A29	A30
1	-0.00111	0.00258	0.00417	-0.00651	0.00228

	A31	A32	A33	A34	A35
1	0.01949	-0.01779	-0.00079	0.02191	-0.00863

	A36	A37	A38	A39	A40
1	-0.01309	-0.00301	0.00683	-0.00385	-0.00110

	A41	A42	A43	A44	A45
1	0.00435	-0.00324	-0.00117	-0.00144	0.00260

	A46	A47	A48	A49	A50
1	0.00417	-0.00631	0.00204	-0.00313	0.00310

	A51	A52	A53	A54	A55

This journal is © The Royal Society of Chemistry 2014

	1	0.00003	-0.00586	0.00300	0.00294	-
0.01368						
		A56	A57	A58	D1	D2
	1	-0.00066	0.00856	-0.00808	0.13678	-
0.00979						
		D3	D4	D5	D6	D7
	1	0.13650	-0.01007	0.01418	0.00233	
0.01446						
		D8	D9	D10	D11	D12
	1	0.00262	0.00017	0.00006	-0.00072	-
0.00083						
		D13	D14	D15	D16	D17
	1	-0.13751	-0.13323	0.01361	0.01789	
0.10891						
		D18	D19	D20	D21	D22
	1	0.11238	-0.04937	-0.04590	0.05241	-
0.15591						
		D23	D24	D25	D26	D27
	1	0.06529	-0.14303	-0.00263	0.00194	-
0.01679						
		D28	D29	D30	D31	D32
	1	-0.01222	0.15497	0.14384	-0.05564	-
0.06676						
		D33	D34	D35	D36	D37
	1	0.00425	0.17468	-0.17299	-0.00256	-
0.14699						
		D38	D39	D40	D41	D42
	1	-0.15133	0.02743	0.02309	-0.02268	-
0.01948						
		D43	D44	D45	D46	D47
	1	0.14559	0.14880	-0.00146	-0.00138	-
0.00154						
		D48	D49	D50	D51	D52
	1	-0.00145	-0.00030	0.00151	-0.00021	
0.00160						
		D53	D54	D55	D56	D57
	1	0.00054	-0.00417	0.00236	-0.00235	-
0.01149						
		D58	D59	D60	D61	D62
	1	-0.01554	-0.00164	-0.00570	0.01484	
0.01002						
		D63	D64	D65	D66	D67
	1	0.00233	-0.00249	0.00285	-0.00055	
0.00814						
		D68	D69	D70	D71	D72
	1	0.00474	0.00203	-0.00012	-0.00141	-
0.00356						
		D73	D74	D75	D76	D77
	1	0.00124	-0.00321	-0.00092	-0.00537	
0.00210						
		D78	D79	D80	D81	D82

```
         1              0.00710  -0.00236   0.00264   0.04234
0.03951
                          D83       D84
         1             -0.04543  -0.04148
 RFO step:  Lambda0=3.934901419D-06 Lambda=-3.21617555D-04.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.02389770 RMS(Int)=  0.00091247
 Iteration  2 RMS(Cart)=  0.00113738 RMS(Int)=  0.00017374
 Iteration  3 RMS(Cart)=  0.00000172 RMS(Int)=  0.00017373
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00017373
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.75079   0.00024   0.00000  -0.00279  -0.00279
2.74800
    R2        2.68958  -0.00014   0.00000  -0.00078  -0.00071
2.68887
    R3        5.47051   0.00026   0.00000   0.05029   0.05033
5.52084
    R4        2.67694  -0.00021   0.00000   0.00013   0.00012
2.67706
    R5        4.45015   0.00008   0.00000   0.09394   0.09411
4.54426
    R6        4.86746   0.00010   0.00000   0.06812   0.06830
4.93576
    R7        2.75056   0.00086   0.00000  -0.00076  -0.00133
2.74923
    R8        2.81975  -0.00033   0.00000  -0.00294  -0.00317
2.81658
    R9        2.72760   0.00034   0.00000   0.00304   0.00310
2.73071
   R10        5.21631   0.00000   0.00000  -0.01836  -0.01840
5.19790
   R11        2.66579  -0.00011   0.00000  -0.00102  -0.00103
2.66476
   R12        2.05792  -0.00010   0.00000  -0.00035  -0.00032
2.05760
   R13        3.92224  -0.00021   0.00000  -0.04771  -0.04775
3.87448
   R14        4.55037  -0.00015   0.00000  -0.03464  -0.03467
4.51570
   R15        2.73431   0.00020   0.00000   0.00287   0.00298
2.73729
   R16        4.73913  -0.00013   0.00000  -0.04786  -0.04792
4.69121
   R17        2.04748   0.00011   0.00000   0.00065   0.00065
2.04813
   R18        2.66852   0.00058   0.00000   0.00097   0.00093
2.66944
   R19        5.05416  -0.00006   0.00000  -0.01846  -0.01840
5.03576
```

This journal is © The Royal Society of Chemistry 2014

R20	2.81883	0.00005	0.00000	0.00542	0.00542
2.82425					
R21	5.14342	-0.00020	0.00000	-0.00851	-0.00845
5.13497					
R22	2.04263	0.00017	0.00000	0.00010	0.00005
2.04268					
R23	5.34168	0.00038	0.00000	0.05925	0.05911
5.40079					
R24	2.79067	0.00010	0.00000	-0.00578	-0.00577
2.78490					
R25	5.32643	0.00027	0.00000	0.04019	0.04017
5.36661					
R26	5.29659	-0.00017	0.00000	0.04272	0.04249
5.33907					
R27	2.04901	0.00005	0.00000	0.00043	0.00043
2.04944					
R28	2.61835	0.00006	0.00000	-0.00021	-0.00021
2.61814					
R29	2.05321	0.00000	0.00000	0.00000	0.00000
2.05320					
R30	2.66252	-0.00007	0.00000	0.00024	0.00025
2.66277					
R31	2.05283	-0.00001	0.00000	-0.00001	-0.00001
2.05282					
R32	2.61589	0.00013	0.00000	0.00079	0.00080
2.61669					
R33	2.05372	-0.00001	0.00000	-0.00012	-0.00012
2.05360					
R34	2.68768	0.00004	0.00000	0.00143	0.00128
2.68896					
R35	2.66299	-0.00003	0.00000	-0.00076	-0.00075
2.66224					
R36	2.67397	0.00025	0.00000	0.00192	0.00153
2.67551					
R37	2.04474	-0.00008	0.00000	-0.00073	-0.00049
2.04425					
R38	2.62190	0.00000	0.00000	-0.00020	-0.00021
2.62169					
R39	4.14188	0.00132	0.00000	0.04713	0.04762
4.18950					
R40	2.05369	-0.00001	0.00000	0.00000	0.00000
2.05369					
R41	2.66216	-0.00011	0.00000	-0.00033	-0.00019
2.66197					
R42	2.05359	0.00000	0.00000	0.00000	0.00000
2.05358					
R43	2.61956	-0.00008	0.00000	0.00002	0.00017
2.61973					
R44	2.05536	-0.00001	0.00000	0.00005	0.00005
2.05541					
R45	2.65486	0.00007	0.00000	0.00417	0.00415
2.65900					

This journal is © The Royal Society of Chemistry 2014

R46	2.27338	0.00012	0.00000	0.00060	0.00060
2.27398					
R47	2.62592	0.00012	0.00000	-0.00371	-0.00374
2.62218					
R48	2.27243	0.00010	0.00000	0.00005	0.00005
2.27248					
R49	2.07980	0.00121	0.00000	0.00485	0.00485
2.08465					
R50	2.30880	-0.00161	0.00000	-0.00173	-0.00161
2.30719					
A1	2.03680	0.00000	0.00000	0.00345	0.00341
2.04020					
A2	2.17959	-0.00017	0.00000	-0.00510	-0.00509
2.17450					
A3	2.06632	0.00018	0.00000	0.00192	0.00192
2.06824					
A4	2.04849	0.00003	0.00000	0.00337	0.00330
2.05179					
A5	2.06574	0.00003	0.00000	-0.00392	-0.00350
2.06224					
A6	2.12366	-0.00003	0.00000	0.01227	0.01109
2.13475					
A7	2.03416	0.00007	0.00000	-0.00118	-0.00120
2.03296					
A8	2.10103	-0.00008	0.00000	-0.00086	-0.00087
2.10016					
A9	2.14559	0.00000	0.00000	0.00184	0.00186
2.14746					
A10	2.04203	-0.00004	0.00000	-0.00274	-0.00278
2.03925					
A11	2.04476	0.00007	0.00000	-0.00347	-0.00355
2.04121					
A12	2.05030	-0.00006	0.00000	-0.00335	-0.00337
2.04693					
A13	2.16092	0.00000	0.00000	-0.00569	-0.00582
2.15509					
A14	2.05949	-0.00006	0.00000	-0.00436	-0.00446
2.05503					
A15	1.85823	-0.00003	0.00000	-0.00419	-0.00420
1.85403					
A16	2.20399	0.00005	0.00000	0.00585	0.00554
2.20953					
A17	1.87541	-0.00009	0.00000	0.00386	0.00382
1.87924					
A18	2.09741	0.00006	0.00000	0.00434	0.00419
2.10160					
A19	2.10509	0.00003	0.00000	-0.00123	-0.00123
2.10386					
A20	2.10055	-0.00006	0.00000	-0.00107	-0.00108
2.09947					
A21	2.07698	0.00003	0.00000	0.00221	0.00221
2.07919					

This journal is © The Royal Society of Chemistry 2014

A22	2.08476	0.00001	0.00000	0.00048	0.00048
2.08524					
A23	2.10896	-0.00004	0.00000	-0.00046	-0.00046
2.10851					
A24	2.08946	0.00003	0.00000	-0.00002	-0.00002
2.08944					
A25	2.09325	-0.00001	0.00000	-0.00045	-0.00046
2.09279					
A26	2.09382	0.00000	0.00000	0.00077	0.00078
2.09459					
A27	2.09612	0.00001	0.00000	-0.00032	-0.00032
2.09580					
A28	2.09483	0.00000	0.00000	-0.00022	-0.00022
2.09461					
A29	2.08244	-0.00001	0.00000	0.00034	0.00034
2.08279					
A30	2.10581	0.00001	0.00000	-0.00011	-0.00011
2.10570					
A31	2.03884	0.00001	0.00000	0.00189	0.00178
2.04062					
A32	2.14033	-0.00001	0.00000	-0.00241	-0.00209
2.13825					
A33	2.10017	-0.00001	0.00000	0.00035	0.00014
2.10031					
A34	2.03148	-0.00011	0.00000	-0.00084	-0.00057
2.03091					
A35	2.17926	0.00019	0.00000	0.00207	0.00137
2.18063					
A36	2.07140	-0.00008	0.00000	-0.00109	-0.00066
2.07073					
A37	2.08192	-0.00029	0.00000	0.00207	0.00171
2.08363					
A38	2.09574	-0.00001	0.00000	-0.00010	-0.00022
2.09553					
A39	2.10548	0.00030	0.00000	-0.00199	-0.00152
2.10396					
A40	2.08356	0.00001	0.00000	-0.00059	-0.00055
2.08301					
A41	2.11086	0.00000	0.00000	0.00075	0.00065
2.11151					
A42	2.08876	-0.00001	0.00000	-0.00015	-0.00010
2.08866					
A43	2.09456	-0.00001	0.00000	0.00033	0.00029
2.09485					
A44	2.09261	0.00004	0.00000	-0.00043	-0.00036
2.09225					
A45	2.09602	-0.00003	0.00000	0.00010	0.00007
2.09609					
A46	2.09464	0.00006	0.00000	0.00054	0.00047
2.09512					
A47	2.08366	-0.00002	0.00000	-0.00027	-0.00024
2.08342					

This journal is © The Royal Society of Chemistry 2014

A48	2.10462	-0.00003	0.00000	-0.00027	-0.00023	2.10438
A49	1.88378	0.00002	0.00000	-0.00084	-0.00083	1.88295
A50	2.28558	0.00001	0.00000	0.00288	0.00288	2.28846
A51	2.11382	-0.00003	0.00000	-0.00205	-0.00205	2.11177
A52	1.88720	-0.00001	0.00000	0.00082	0.00082	1.88803
A53	2.26412	-0.00001	0.00000	-0.00288	-0.00289	2.26124
A54	2.13169	0.00002	0.00000	0.00201	0.00201	2.13370
A55	1.90736	0.00010	0.00000	0.00018	0.00015	1.90751
A56	2.01367	-0.00035	0.00000	-0.01141	-0.01104	2.00262
A57	2.18101	0.00034	0.00000	0.00966	0.00893	2.18994
A58	2.08661	0.00005	0.00000	0.00188	0.00224	2.08885
D1	-0.58575	0.00012	0.00000	0.01412	0.01420	-0.57155
D2	2.86898	0.00007	0.00000	-0.02743	-0.02683	2.84216
D3	2.58969	0.00010	0.00000	0.00441	0.00438	2.59407
D4	-0.23876	0.00004	0.00000	-0.03714	-0.03664	-0.27540
D5	-0.01338	-0.00001	0.00000	-0.01442	-0.01441	-0.02779
D6	-3.08277	-0.00002	0.00000	-0.01137	-0.01145	-3.09421
D7	3.09665	0.00000	0.00000	-0.00551	-0.00536	3.09129
D8	0.02726	-0.00001	0.00000	-0.00247	-0.00240	0.02487
D9	-0.06330	0.00004	0.00000	0.00783	0.00788	-0.05542
D10	3.11479	0.00003	0.00000	0.01080	0.01082	3.12561
D11	3.11266	0.00002	0.00000	-0.00206	-0.00210	3.11056
D12	0.00757	0.00001	0.00000	0.00091	0.00084	0.00840
D13	0.57274	-0.00016	0.00000	-0.00951	-0.00955	0.56319
D14	-2.61893	-0.00014	0.00000	-0.00612	-0.00622	-2.62515
D15	-2.89303	-0.00009	0.00000	0.03036	0.03044	-2.86259

This journal is © The Royal Society of Chemistry 2014

D16	0.19848	-0.00007	0.00000	0.03374	0.03377	0.23226
D17	-0.28601	0.00003	0.00000	-0.07356	-0.07363	-0.35964
D18	2.92246	-0.00068	0.00000	-0.07581	-0.07597	2.84648
D19	-3.10034	-0.00004	0.00000	-0.11514	-0.11508	3.06776
D20	0.10812	-0.00075	0.00000	-0.11740	-0.11743	-0.00930
D21	-3.08402	-0.00003	0.00000	-0.01006	-0.01013	-3.09415
D22	0.62500	0.00003	0.00000	0.00779	0.00767	0.63266
D23	-0.01666	-0.00002	0.00000	-0.01332	-0.01330	-0.02996
D24	-2.59082	0.00004	0.00000	0.00453	0.00449	-2.58634
D25	-0.04357	0.00000	0.00000	0.00156	0.00153	-0.04204
D26	3.11336	0.00000	0.00000	0.00061	0.00061	3.11397
D27	-3.10819	-0.00001	0.00000	0.00494	0.00484	-3.10336
D28	0.04874	-0.00002	0.00000	0.00399	0.00391	0.05266
D29	-0.63812	-0.00001	0.00000	-0.00286	-0.00279	-0.64091
D30	2.59732	0.00002	0.00000	-0.00090	-0.00080	2.59653
D31	3.07362	0.00004	0.00000	0.01489	0.01488	3.08851
D32	0.02588	0.00007	0.00000	0.01684	0.01688	0.04276
D33	-0.13082	-0.00021	0.00000	-0.04242	-0.04241	-0.17322
D34	2.52505	-0.00015	0.00000	-0.01154	-0.01147	2.51358
D35	-2.60786	-0.00005	0.00000	-0.02087	-0.02093	-2.62878
D36	0.04801	0.00001	0.00000	0.01001	0.01001	0.05802
D37	-2.64838	0.00012	0.00000	0.01365	0.01363	-2.63475
D38	0.51318	0.00012	0.00000	0.01642	0.01640	0.52958
D39	-0.12593	0.00000	0.00000	-0.00702	-0.00700	-0.13294
D40	3.03563	0.00000	0.00000	-0.00425	-0.00423	3.03140
D41	0.04438	-0.00001	0.00000	-0.01004	-0.01005	0.03433

This journal is © The Royal Society of Chemistry 2014

D42	-3.09680	-0.00008	0.00000	-0.00757	-0.00755	-3.10435
D43	2.73557	0.00005	0.00000	0.01910	0.01906	2.75463
D44	-0.40561	-0.00002	0.00000	0.02158	0.02155	-0.38406
D45	3.11596	0.00000	0.00000	-0.00038	-0.00035	3.11561
D46	-0.02660	0.00001	0.00000	0.00160	0.00163	-0.02497
D47	0.01028	-0.00001	0.00000	0.00262	0.00262	0.01290
D48	-3.13228	0.00000	0.00000	0.00459	0.00460	-3.12768
D49	-3.13094	0.00000	0.00000	-0.00189	-0.00190	-3.13284
D50	0.01045	-0.00002	0.00000	-0.00256	-0.00254	0.00792
D51	0.00968	0.00001	0.00000	0.00009	0.00009	0.00977
D52	-3.13211	-0.00001	0.00000	-0.00058	-0.00055	-3.13266
D53	0.02464	0.00001	0.00000	0.00099	0.00097	0.02560
D54	-3.13251	0.00001	0.00000	0.00196	0.00190	-3.13060
D55	-3.11715	0.00000	0.00000	0.00032	0.00032	-3.11683
D56	0.00889	0.00000	0.00000	0.00128	0.00126	0.01015
D57	0.03539	0.00011	0.00000	0.00448	0.00449	0.03988
D58	-3.05936	0.00008	0.00000	0.00122	0.00132	-3.05805
D59	3.08542	0.00008	0.00000	0.00241	0.00241	3.08783
D60	-0.00933	0.00005	0.00000	-0.00085	-0.00076	-0.01009
D61	3.08245	-0.00005	0.00000	-0.00161	-0.00168	3.08076
D62	-0.08358	-0.00004	0.00000	-0.00171	-0.00176	-0.08534
D63	0.03790	-0.00002	0.00000	0.00035	0.00030	0.03820
D64	-3.12813	-0.00001	0.00000	0.00025	0.00023	-3.12790
D65	0.03475	-0.00020	0.00000	0.00053	0.00047	0.03522
D66	-3.11700	-0.00006	0.00000	-0.00205	-0.00207	-3.11907
D67	3.12521	-0.00018	0.00000	0.00399	0.00388	3.12909

```
   D68       -0.02655  -0.00003   0.00000   0.00142   0.00134  -
0.02521
   D69       -3.10952  -0.00002   0.00000   0.00030   0.00030  -
3.10922
   D70        0.03452   0.00000   0.00000  -0.00145  -0.00144
0.03308
   D71        0.02177   0.00012   0.00000  -0.00229  -0.00225
0.01952
   D72       -3.11737   0.00014   0.00000  -0.00404  -0.00400  -
3.12137
   D73        3.13754   0.00000   0.00000   0.00131   0.00130
3.13884
   D74       -0.00578   0.00003   0.00000   0.00091   0.00095  -
0.00483
   D75       -0.00160   0.00002   0.00000  -0.00045  -0.00045  -
0.00205
   D76        3.13827   0.00004   0.00000  -0.00084  -0.00080
3.13746
   D77       -0.03043  -0.00002   0.00000  -0.00036  -0.00038  -
0.03081
   D78        3.13590  -0.00003   0.00000  -0.00026  -0.00031
3.13559
   D79        3.10944   0.00001   0.00000  -0.00075  -0.00074
3.10870
   D80       -0.00742   0.00000   0.00000  -0.00065  -0.00067  -
0.00809
   D81       -0.12633   0.00000   0.00000   0.00544   0.00543  -
0.12090
   D82        3.01490   0.00006   0.00000   0.00326   0.00325
3.01814
   D83        0.15633   0.00001   0.00000   0.00088   0.00088
0.15721
   D84       -3.00340   0.00001   0.00000  -0.00171  -0.00171  -
3.00511
         Item               Value     Threshold  Converged?
 Maximum Force            0.001614     0.000450     NO
 RMS     Force            0.000228     0.000300     YES
 Maximum Displacement     0.169616     0.001800     NO
 RMS     Displacement     0.023815     0.001200     NO
 Predicted change in Energy=-1.720920D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.556457    0.522262    1.162519
    2          6             0        0.603239    1.084282    0.488820
    3          6             0       -0.742649   -0.884501    1.057777
```

4	6	0	0.223775	-1.604767	0.260693
5	1	0	0.061207	-2.674493	0.138966
6	6	0	-0.204495	-0.962038	-1.638562
7	1	0	0.490500	-1.644642	-2.113648
8	6	0	-0.095328	0.443914	-1.721298
9	1	0	0.740210	1.003161	-2.118218
10	6	0	-1.513648	1.279117	1.882121
11	1	0	-1.389233	2.349199	2.007108
12	6	0	-2.597544	0.652353	2.475283
13	1	0	-3.310536	1.242340	3.044542
14	6	0	-2.784364	-0.738636	2.349780
15	1	0	-3.643855	-1.213782	2.814076
16	6	0	-1.873729	-1.498007	1.634608
17	1	0	-2.013153	-2.569914	1.522669
18	6	0	1.595858	-1.143986	0.317665
19	6	0	1.800229	0.261179	0.409780
20	6	0	3.124937	0.758781	0.364171
21	1	0	3.293363	1.825824	0.421452
22	6	0	4.194122	-0.119375	0.262243
23	1	0	5.207452	0.273328	0.258716
24	6	0	3.984359	-1.508765	0.162732
25	1	0	4.833181	-2.182384	0.081016
26	6	0	2.693710	-2.014702	0.171765
27	1	0	2.518501	-3.085051	0.089968
28	6	0	-1.460352	0.995609	-1.785767
29	6	0	-1.662800	-1.274194	-1.736172
30	8	0	-2.365151	-0.078179	-1.695186
31	8	0	-2.214366	-2.339960	-1.813874
32	8	0	-1.851755	2.128050	-1.897125
33	6	0	0.629038	2.553770	0.240947
34	1	0	-0.359515	3.042919	0.261695
35	8	0	1.621714	3.208219	-0.036391

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.454177	0.000000			
3	C	1.422891	2.451781	0.000000		
4	C	2.438505	2.725256	1.445027	0.000000	
5	H	3.412977	3.813737	2.166673	1.088833	0.000000
6	C	3.189526	3.060329	2.750612	2.050289	2.482480
7	H	4.065078	3.772608	3.486604	2.389608	2.513794
8	C	2.921503	2.404721	3.147533	2.868311	3.634494
9	H	3.560316	2.611893	3.981091	3.567522	4.368188
10	C	1.416641	2.541743	2.440332	3.736905	4.598890
11	H	2.178198	2.806271	3.431634	4.613633	5.552586
12	C	2.430290	3.791782	2.794973	4.237787	4.857493
13	H	3.412547	4.677001	3.881331	5.324208	5.928963
14	C	2.821883	4.273413	2.420568	3.763425	4.090540
15	H	3.908134	5.359638	3.407346	4.650935	4.797643
16	C	2.457551	3.757182	1.410129	2.509694	2.713861
17	H	3.437037	4.611670	2.161232	2.743709	2.495704

This journal is © The Royal Society of Chemistry 2014

18	C	2.850021	2.445356	2.466519	1.448509	2.174751
19	C	2.487720	1.454830	2.863340	2.447283	3.422822
20	C	3.774382	2.545672	4.259071	3.743503	4.607009
21	H	4.131533	2.791271	4.903077	4.606211	5.547926
22	C	4.877519	3.794018	5.058656	4.239110	4.860536
23	H	5.839646	4.680745	6.114145	5.325813	5.931932
24	C	5.073820	4.273430	4.851332	3.763085	4.092751
25	H	6.126415	5.360021	5.807620	4.648931	4.797631
26	C	4.240444	3.751573	3.724371	2.505302	2.714125
27	H	4.859880	4.605502	4.051441	2.736084	2.491837
28	C	3.119852	3.072460	3.483626	3.712982	4.414679
29	C	3.585200	3.955747	2.967270	2.766932	2.906748
30	O	3.434877	3.864264	3.295675	3.585871	3.999022
31	O	4.449707	4.996671	3.539871	3.284640	3.017239
32	O	3.690227	3.578991	4.363143	4.785178	5.556034
33	C	2.526206	1.490470	3.790836	4.178284	5.259997
34	H	2.684024	2.194251	4.025563	4.684145	5.734184
35	O	3.660079	2.413348	4.851574	5.020691	6.088697

		6	7	8	9	10
6	C	0.000000				
7	H	1.083823	0.000000			
8	C	1.412609	2.204359	0.000000		
9	H	2.232610	2.659556	1.080938	0.000000	
10	C	4.373999	5.341455	3.961543	4.599864	0.000000
11	H	5.065452	6.038608	4.382386	4.833700	1.084517
12	C	5.025601	5.989198	4.890381	5.688930	1.385462
13	H	6.036409	7.027763	5.804160	6.566570	2.140416
14	C	4.755261	5.609614	5.020260	5.951428	2.429970
15	H	5.631923	6.446782	5.992463	6.961493	3.408939
16	C	3.713118	4.434016	4.265662	5.212698	2.811287
17	H	3.981192	4.510788	4.825405	5.796890	3.897916
18	C	2.664808	2.717308	3.088512	3.357961	4.241223
19	C	3.116230	3.422753	2.857975	2.839886	3.766400
20	C	4.249385	4.342383	3.849471	3.450927	4.908298
21	H	4.924515	5.130976	4.240788	3.693953	5.053692
22	C	4.865283	4.657050	4.759319	4.342372	6.095771
23	H	5.866427	5.617505	5.662952	5.112604	6.987148
24	C	4.592393	4.172221	4.899630	4.694360	6.399740
25	H	5.461170	4.895366	5.868218	5.633537	7.450383
26	C	3.575610	3.195966	4.172196	4.262357	5.610386
27	H	3.861309	3.323175	4.750408	4.975126	6.206126
28	C	2.330500	3.299129	1.473707	2.225546	3.679215
29	C	1.494531	2.217300	2.325744	3.332682	4.430992
30	O	2.335133	3.283848	2.329240	3.315346	3.919750
31	O	2.443150	2.808848	3.499835	4.471980	5.220067
32	O	3.511262	4.445924	2.439726	2.834174	3.888149
33	C	4.072866	4.815597	2.970960	2.825316	2.984844
34	H	4.435616	5.323345	3.279768	3.321745	2.658722
35	O	4.826287	5.398602	3.664496	3.158059	4.151219

		11	12	13	14	15
11	H	0.000000				
12	C	2.135063	0.000000			

13	H	2.448023	1.086507	0.000000		
14	C	3.405663	1.409079	2.164213	0.000000	
15	H	4.292942	2.166103	2.489327	1.086305	0.000000
16	C	3.895444	2.419646	3.400268	1.384692	2.145990
17	H	4.982131	3.410570	4.304948	2.152314	2.483146
18	C	4.895643	5.046461	6.099435	4.845632	5.804441
19	C	4.133274	4.874396	5.833059	5.077571	6.131411
20	C	5.060276	6.100402	6.988099	6.411298	7.463885
21	H	4.971411	6.348074	7.129694	6.872676	7.942849
22	C	6.349194	7.184695	8.118827	7.310306	8.315255
23	H	7.133187	8.122486	9.014207	8.322604	9.332041
24	C	6.867394	7.303408	8.311974	7.154851	8.081231
25	H	7.934955	8.305656	9.318334	8.078286	8.959238
26	C	6.251603	6.357417	7.410273	6.031699	6.912888
27	H	6.962534	6.769921	7.837952	6.223567	6.992642
28	C	4.027798	4.423526	5.178411	4.675827	5.550464
29	C	5.216892	4.724583	5.648292	4.270800	4.963163
30	O	4.533383	4.240342	5.010243	4.119914	4.822667
31	O	6.104830	5.243818	6.135035	4.497238	4.972890
32	O	3.937749	4.674595	5.228058	5.208056	6.047716
33	C	2.689719	4.361018	5.010014	5.190224	6.250844
34	H	2.141969	3.952664	4.437888	4.953802	5.951557
35	O	3.738931	5.535621	6.138723	6.378480	7.443485

		16	17	18	19	20
16	C	0.000000				
17	H	1.086717	0.000000			
18	C	3.727962	4.063283	0.000000		
19	C	4.253576	4.878063	1.422934	0.000000	
20	C	5.629721	6.230754	2.441468	1.415817	0.000000
21	H	6.262463	6.978130	3.422289	2.162799	1.081771
22	C	6.372035	6.791471	2.793542	2.428438	1.387338
23	H	7.427908	7.862489	3.880188	3.410591	2.140947
24	C	6.040176	6.240643	2.421158	2.822084	2.433301
25	H	6.918429	7.007199	3.408011	3.908694	3.413024
26	C	4.823731	4.928262	1.408799	2.456542	2.813394
27	H	4.918974	4.780574	2.161215	3.437361	3.901025
28	C	4.252995	4.895333	4.282840	3.998900	5.069832
29	C	3.384781	3.524441	3.854096	4.353741	5.609533
30	O	3.653072	4.085001	4.569147	4.679363	5.923049
31	O	3.566083	3.350505	4.526767	5.275181	6.546314
32	O	5.061808	5.813080	5.243811	4.705742	5.635230
33	C	4.962159	5.905600	3.822829	2.579954	3.076797
34	H	4.979733	5.985688	4.621340	3.524840	4.167636
35	O	6.095812	7.002125	4.366659	2.985964	2.901702

		21	22	23	24	25
21	H	0.000000				
22	C	2.149538	0.000000			
23	H	2.469911	1.086768	0.000000		
24	C	3.415245	1.408654	2.163567	0.000000	
25	H	4.307281	2.167313	2.490417	1.086710	0.000000
26	C	3.895070	2.419026	3.400226	1.386301	2.147950
27	H	4.982669	3.410663	4.305536	2.153767	2.484479

This journal is © The Royal Society of Chemistry 2014

28	C	5.306494	6.116422	7.011505	6.301859	7.293359
29	C	6.231293	6.295301	7.319479	5.962489	6.806230
30	O	6.334364	6.845238	7.828512	6.768657	7.707046
31	O	7.258479	7.092953	8.136847	6.559120	7.299545
32	O	5.651493	6.801942	7.610522	7.178417	8.196417
33	C	2.767872	4.456005	5.114939	5.269581	6.334947
34	H	3.853617	5.543980	6.217858	6.292604	7.368890
35	O	2.216990	4.216557	4.643080	5.279364	6.275820

		26	27	28	29	30
26	C	0.000000				
27	H	1.087674	0.000000			
28	C	5.490915	6.000120	0.000000		
29	C	4.813290	4.908897	2.279353	0.000000	
30	O	5.729547	6.006505	1.407084	1.387598	0.000000
31	O	5.304504	5.155560	3.419846	1.202547	2.269906
32	O	6.488756	7.086896	1.203337	3.411286	2.274159
33	C	5.013841	5.948879	3.301664	4.880044	4.431809
34	H	5.908452	6.772332	3.097647	4.932290	4.194426
35	O	5.335861	6.358100	4.177929	5.811138	5.426519

		31	32	33	34	35
31	O	0.000000				
32	O	4.483473	0.000000			
33	C	6.021281	3.302563	0.000000		
34	H	6.060019	2.779256	1.103148	0.000000	
35	O	6.975475	4.085840	1.220912	2.010336	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.520928	0.675197	1.090334
2	6	0	0.626590	1.126713	0.319642
3	6	0	-0.724819	-0.730290	1.177817
4	6	0	0.212572	-1.563262	0.459792
5	1	0	0.035449	-2.637294	0.485139
6	6	0	-0.258592	-1.171661	-1.496821
7	1	0	0.416346	-1.920859	-1.894104
8	6	0	-0.136633	0.209288	-1.768061
9	1	0	0.694106	0.699257	-2.256151
10	6	0	-1.450736	1.534044	1.726503
11	1	0	-1.311660	2.609397	1.705279
12	6	0	-2.525294	1.006632	2.424118
13	1	0	-3.216736	1.676758	2.927444
14	6	0	-2.730190	-0.385961	2.488951
15	1	0	-3.582202	-0.783321	3.033230
16	6	0	-1.846829	-1.246060	1.858653

```
   17          1             0       -2.000585   -2.321283    1.893417
   18          6             0        1.590520   -1.118341    0.421288
   19          6             0        1.812233    0.283635    0.321057
   20          6             0        3.140521    0.752135    0.177191
   21          1             0        3.321778    1.814893    0.088200
   22          6             0        4.197221   -0.146740    0.166382
   23          1             0        5.214242    0.227746    0.085806
   24          6             0        3.970092   -1.533985    0.257324
   25          1             0        4.809232   -2.224367    0.244830
   26          6             0        2.674799   -2.016067    0.365215
   27          1             0        2.486081   -3.085251    0.430520
   28          6             0       -1.496912    0.766740   -1.871515
   29          6             0       -1.722209   -1.473446   -1.516181
   30          8             0       -2.410429   -0.272770   -1.616975
   31          8             0       -2.286974   -2.532252   -1.438152
   32          8             0       -1.878994    1.879864   -2.122485
   33          6             0        0.661552    2.549943   -0.121600
   34          1             0       -0.320835    3.051391   -0.141594
   35          8             0        1.653525    3.147888   -0.507707
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3889213      0.2595399
0.2424866
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1907.1930048643 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A)

Harris functional with IExCor= 402 diagonalized for initial guess.
ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV=1
ScaDFX= 1.000000 1.000000 1.000000 1.000000
Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB+HF-LYP) = -1032.13800818 A.U. after 18 cycles
Convg = 0.1258D-08 -V/T = 2.0093
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000034510	-0.000092758	0.000159043
2	6	-0.000640858	-0.000224268	-0.000039795
3	6	0.000020553	0.000102323	0.000007747
4	6	0.000154436	0.000061798	-0.000138848
5	1	-0.000004705	0.000014001	0.000028426
6	6	-0.000059320	-0.000440881	0.000207829
7	1	-0.000013353	-0.000007792	-0.000021540
8	6	0.000005749	0.000385567	0.000125721
9	1	0.000010145	0.000080223	-0.000098161

This journal is © The Royal Society of Chemistry 2014

```
   10          6           0.000078958   -0.000043161   -0.000137331
   11          1           0.000016202    0.000118357   -0.000077839
   12          6          -0.000046220   -0.000034759    0.000031214
   13          1          -0.000000477   -0.000002828   -0.000000324
   14          6          -0.000004747    0.000065614    0.000003943
   15          1          -0.000000696   -0.000001283   -0.000004233
   16          6           0.000052013    0.000012021   -0.000056608
   17          1          -0.000000340   -0.000004918   -0.000010544
   18          6          -0.000055880   -0.000159651    0.000002613
   19          6           0.000149465   -0.000140751    0.000181429
   20          6           0.000364256    0.000006030   -0.000030292
   21          1           0.000240508   -0.000272449   -0.000050377
   22          6           0.000019399    0.000000609   -0.000005412
   23          1           0.000005764   -0.000029094   -0.000005080
   24          6          -0.000129258    0.000060909   -0.000001407
   25          1          -0.000004731    0.000002615    0.000001907
   26          6           0.000109877    0.000074127   -0.000016000
   27          1           0.000014795    0.000002860   -0.000003133
   28          6           0.000080010   -0.000070809   -0.000047060
   29          6           0.000047524    0.000024752   -0.000045345
   30          8          -0.000065221   -0.000040704   -0.000023902
   31          8          -0.000032275   -0.000057708   -0.000001521
   32          8          -0.000021079    0.000101366    0.000055974
   33          6           0.000222737    0.000366977   -0.000524673
   34          1          -0.000030090    0.000095035    0.000200282
   35          8          -0.000448635    0.000048631    0.000333297
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000640858 RMS     0.000148664


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000411067 RMS     0.000093761
 Search for a saddle point.
 Step number   5 out of a maximum of 202
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Update second derivatives using D2CorX and points  3  4  5
     Eigenvalues ---   -0.01911   0.00269   0.00365   0.00732
0.00858
     Eigenvalues ---    0.01084   0.01256   0.01437   0.01469
0.01524
     Eigenvalues ---    0.01602   0.01704   0.01760   0.01801
0.01913
     Eigenvalues ---    0.01974   0.02110   0.02173   0.02191
0.02231
     Eigenvalues ---    0.02359   0.02426   0.02449   0.02515
0.02686
     Eigenvalues ---    0.02727   0.02746   0.02753   0.03255
0.03538
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.04194   0.05547   0.07029   0.07473
0.07789
     Eigenvalues ---    0.08789   0.10192   0.11051   0.11179
0.11225
     Eigenvalues ---    0.11853   0.12290   0.12499   0.12527
0.12660
     Eigenvalues ---    0.12836   0.13907   0.14280   0.14662
0.16368
     Eigenvalues ---    0.17653   0.18504   0.19086   0.19175
0.19334
     Eigenvalues ---    0.19419   0.20110   0.20418   0.20904
0.21162
     Eigenvalues ---    0.23351   0.23904   0.24402   0.25101
0.26054
     Eigenvalues ---    0.27638   0.27936   0.29113   0.30147
0.30311
     Eigenvalues ---    0.31237   0.33091   0.33998   0.34048
0.35021
     Eigenvalues ---    0.35279   0.35919   0.36086   0.36133
0.36202
     Eigenvalues ---    0.36237   0.36329   0.36535   0.37436
0.37826
     Eigenvalues ---    0.38853   0.39868   0.40318   0.41115
0.42459
     Eigenvalues ---    0.44484   0.46388   0.47305   0.47638
0.50257
     Eigenvalues ---    0.50619   0.79400   0.89039
0.902561000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                          R1        R2        R3        R4        R5
          1             -0.04342   0.02341   0.16153   0.01782
0.38301
                          R6        R7        R8        R9        R10
          1              0.11510  -0.04391  -0.01989  -0.06014
0.18793
                          R11       R12       R13       R14       R15
          1              0.01918  -0.00712   0.43335   0.17582  -
0.05864
                          R16       R17       R18       R19       R20
          1              0.28219  -0.00744  -0.09468   0.18082  -
0.01212
                          R21       R22       R23       R24       R25
          1             -0.03038  -0.00731   0.16525  -0.00724  -
0.03285
                          R26       R27       R28       R29       R30
          1              0.07456  -0.00140  -0.01368   0.00007
0.01457
                          R31       R32       R33       R34       R35
          1             -0.00022  -0.01598  -0.00026   0.02099
0.01804
                          R36       R37       R38       R39       R40
          1              0.01738  -0.00168  -0.01223  -0.04782
0.00007
                          R41       R42       R43       R44       R45
          1              0.01330  -0.00013  -0.01526  -0.00014
0.00292
                          R46       R47       R48       R49       R50
          1              0.00094  -0.00259   0.00263  -0.00107
0.00517
                          A1        A2        A3        A4        A5
          1              0.02172  -0.00881  -0.01292   0.03292
0.00002
                          A6        A7        A8        A9        A10
          1              0.00408   0.01878  -0.00165  -0.01623
0.03285
                          A11       A12       A13       A14       A15
```

```
          1              0.05614   0.02924   0.06037   0.04084
0.02163
                           A16       A17       A18       A19       A20
          1              0.04772   0.00806   0.01690  -0.00391
0.00672
                           A21       A22       A23       A24       A25
          1             -0.00279  -0.00116   0.00474  -0.00357  -
0.00144
                           A26       A27       A28       A29       A30
          1             -0.00116   0.00261   0.00417  -0.00653
0.00230
                           A31       A32       A33       A34       A35
          1              0.01939  -0.01774  -0.00071   0.02187  -
0.00847
                           A36       A37       A38       A39       A40
          1             -0.01323  -0.00301   0.00690  -0.00393  -
0.00109
                           A41       A42       A43       A44       A45
          1              0.00435  -0.00326  -0.00117  -0.00145
0.00261
                           A46       A47       A48       A49       A50
          1              0.00416  -0.00631   0.00205  -0.00249
0.00258
                           A51       A52       A53       A54       A55
          1             -0.00010  -0.00643   0.00348   0.00303  -
0.01374
                           A56       A57       A58        D1        D2
          1             -0.00008   0.00819  -0.00825   0.13611  -
0.00753
                            D3        D4        D5        D6        D7
          1              0.13674  -0.00689   0.01555   0.00329
0.01497
                            D8        D9       D10       D11       D12
          1              0.00272  -0.00056  -0.00102  -0.00035  -
0.00081
                           D13       D14       D15       D16       D17
          1             -0.13737  -0.13353   0.01223   0.01607
0.11452
                           D18       D19       D20       D21       D22
          1              0.11758  -0.04103  -0.03797   0.05252  -
0.15645
                           D23       D24       D25       D26       D27
          1              0.06589  -0.14308  -0.00270   0.00197  -
0.01740
                           D28       D29       D30       D31       D32
          1             -0.01273   0.15494   0.14364  -0.05625  -
0.06755
                           D33       D34       D35       D36       D37
          1              0.00598   0.17533  -0.17205  -0.00271  -
0.14800
                           D38       D39       D40       D41       D42
```

```
          1             -0.15237   0.02756   0.02320  -0.02240  -
0.01933
                           D43       D44       D45       D46       D47
          1              0.14423   0.14731  -0.00144  -0.00153  -
0.00186
                           D48       D49       D50       D51       D52
          1             -0.00195  -0.00017   0.00167  -0.00027
0.00158
                           D53       D54       D55       D56       D57
          1              0.00048  -0.00432   0.00233  -0.00248  -
0.01189
                           D58       D59       D60       D61       D62
          1             -0.01554  -0.00187  -0.00552   0.01496
0.01016
                           D63       D64       D65       D66       D67
          1              0.00226  -0.00255   0.00287  -0.00024
0.00766
                           D68       D69       D70       D71       D72
          1              0.00454   0.00201   0.00001  -0.00114  -
0.00314
                           D73       D74       D75       D76       D77
          1              0.00115  -0.00324  -0.00086  -0.00525
0.00211
                           D78       D79       D80       D81       D82
          1              0.00709  -0.00230   0.00269   0.04207
0.03937
                           D83       D84
          1             -0.04560  -0.04160
 RFO step:  Lambda0=8.505540630D-07 Lambda=-1.65085156D-05.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.00474532 RMS(Int)=  0.00001048
 Iteration  2 RMS(Cart)=  0.00001350 RMS(Int)=  0.00000192
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000192
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.74800  -0.00019   0.00000  -0.00065  -0.00065
2.74735
    R2        2.68887  -0.00012   0.00000  -0.00026  -0.00026
2.68861
    R3        5.52084  -0.00010   0.00000   0.00210   0.00210
5.52294
    R4        2.67706  -0.00015   0.00000   0.00010   0.00010
2.67716
    R5        4.54426  -0.00007   0.00000   0.00946   0.00946
4.55372
    R6        4.93576  -0.00007   0.00000   0.00903   0.00903
4.94480
    R7        2.74923   0.00041   0.00000   0.00131   0.00130
2.75053
    R8        2.81658   0.00025   0.00000   0.00159   0.00159
2.81817
```

This journal is © The Royal Society of Chemistry 2014

R9	2.73071	0.00014	0.00000	-0.00013	-0.00013
2.73058					
R10	5.19790	0.00000	0.00000	-0.00200	-0.00200
5.19590					
R11	2.66476	-0.00005	0.00000	-0.00003	-0.00003
2.66473					
R12	2.05760	0.00003	0.00000	-0.00004	-0.00004
2.05756					
R13	3.87448	-0.00003	0.00000	-0.00169	-0.00169
3.87279					
R14	4.51570	0.00004	0.00000	-0.00122	-0.00122
4.51449					
R15	2.73729	-0.00006	0.00000	-0.00055	-0.00055
2.73674					
R16	4.69121	-0.00008	0.00000	-0.00215	-0.00215
4.68905					
R17	2.04813	0.00000	0.00000	0.00001	0.00001
2.04814					
R18	2.66944	0.00041	0.00000	0.00060	0.00060
2.67005					
R19	5.03576	0.00003	0.00000	-0.00101	-0.00101
5.03475					
R20	2.82425	0.00000	0.00000	0.00026	0.00026
2.82451					
R21	5.13497	-0.00003	0.00000	-0.00126	-0.00126
5.13371					
R22	2.04268	0.00010	0.00000	0.00018	0.00018
2.04286					
R23	5.40079	0.00008	0.00000	0.00717	0.00717
5.40796					
R24	2.78490	-0.00002	0.00000	-0.00069	-0.00069
2.78422					
R25	5.36661	0.00005	0.00000	0.00832	0.00832
5.37492					
R26	5.33907	0.00005	0.00000	0.01526	0.01526
5.35434					
R27	2.04944	0.00011	0.00000	0.00014	0.00014
2.04958					
R28	2.61814	0.00002	0.00000	-0.00009	-0.00009
2.61806					
R29	2.05320	0.00000	0.00000	-0.00001	-0.00001
2.05319					
R30	2.66277	-0.00001	0.00000	0.00004	0.00005
2.66282					
R31	2.05282	0.00000	0.00000	0.00000	0.00000
2.05282					
R32	2.61669	0.00008	0.00000	0.00003	0.00003
2.61671					
R33	2.05360	0.00000	0.00000	0.00001	0.00001
2.05361					
R34	2.68896	0.00002	0.00000	0.00047	0.00047
2.68942					

This journal is © The Royal Society of Chemistry 2014

R35	2.66224	-0.00001	0.00000	0.00010	0.00010
2.66235					
R36	2.67551	0.00031	0.00000	0.00114	0.00114
2.67664					
R37	2.04425	-0.00006	0.00000	-0.00042	-0.00042
2.04384					
R38	2.62169	-0.00005	0.00000	-0.00022	-0.00022
2.62147					
R39	4.18950	0.00036	0.00000	0.00829	0.00830
4.19780					
R40	2.05369	-0.00001	0.00000	-0.00002	-0.00002
2.05367					
R41	2.66197	-0.00008	0.00000	-0.00015	-0.00015
2.66183					
R42	2.05358	-0.00001	0.00000	-0.00001	-0.00001
2.05358					
R43	2.61973	-0.00010	0.00000	-0.00050	-0.00050
2.61923					
R44	2.05541	0.00000	0.00000	0.00000	0.00000
2.05541					
R45	2.65900	0.00009	0.00000	0.00052	0.00052
2.65952					
R46	2.27398	0.00010	0.00000	0.00018	0.00018
2.27416					
R47	2.62218	0.00003	0.00000	-0.00024	-0.00024
2.62194					
R48	2.27248	0.00007	0.00000	0.00010	0.00010
2.27259					
R49	2.08465	0.00007	0.00000	0.00013	0.00013
2.08478					
R50	2.30719	-0.00033	0.00000	-0.00057	-0.00057
2.30662					
A1	2.04020	-0.00005	0.00000	0.00040	0.00039
2.04060					
A2	2.17450	-0.00014	0.00000	-0.00066	-0.00066
2.17384					
A3	2.06824	0.00019	0.00000	0.00021	0.00020
2.06845					
A4	2.05179	0.00012	0.00000	0.00113	0.00113
2.05292					
A5	2.06224	-0.00003	0.00000	-0.00115	-0.00114
2.06110					
A6	2.13475	-0.00010	0.00000	0.00019	0.00018
2.13493					
A7	2.03296	0.00005	0.00000	0.00005	0.00005
2.03301					
A8	2.10016	-0.00010	0.00000	-0.00013	-0.00013
2.10003					
A9	2.14746	0.00005	0.00000	-0.00007	-0.00007
2.14739					
A10	2.03925	-0.00004	0.00000	-0.00042	-0.00042
2.03883					

This journal is © The Royal Society of Chemistry 2014

A11	2.04121	0.00010	0.00000	0.00080	0.00080
2.04201					
A12	2.04693	-0.00004	0.00000	-0.00025	-0.00025
2.04668					
A13	2.15509	0.00003	0.00000	-0.00025	-0.00025
2.15484					
A14	2.05503	-0.00004	0.00000	-0.00058	-0.00058
2.05444					
A15	1.85403	-0.00001	0.00000	-0.00045	-0.00045
1.85358					
A16	2.20953	0.00009	0.00000	0.00097	0.00097
2.21049					
A17	1.87924	-0.00007	0.00000	0.00021	0.00021
1.87945					
A18	2.10160	-0.00003	0.00000	-0.00014	-0.00014
2.10146					
A19	2.10386	-0.00002	0.00000	-0.00001	-0.00001
2.10385					
A20	2.09947	-0.00006	0.00000	-0.00004	-0.00004
2.09943					
A21	2.07919	0.00008	0.00000	0.00009	0.00009
2.07928					
A22	2.08524	0.00003	0.00000	0.00008	0.00008
2.08532					
A23	2.10851	-0.00006	0.00000	-0.00014	-0.00014
2.10836					
A24	2.08944	0.00003	0.00000	0.00006	0.00006
2.08950					
A25	2.09279	-0.00002	0.00000	-0.00004	-0.00004
2.09276					
A26	2.09459	0.00003	0.00000	0.00009	0.00009
2.09468					
A27	2.09580	-0.00002	0.00000	-0.00005	-0.00005
2.09574					
A28	2.09461	-0.00001	0.00000	0.00004	0.00004
2.09464					
A29	2.08279	0.00000	0.00000	-0.00001	-0.00001
2.08278					
A30	2.10570	0.00001	0.00000	-0.00002	-0.00002
2.10568					
A31	2.04062	-0.00005	0.00000	0.00042	0.00042
2.04104					
A32	2.13825	0.00007	0.00000	-0.00090	-0.00090
2.13735					
A33	2.10031	-0.00002	0.00000	0.00040	0.00040
2.10071					
A34	2.03091	-0.00008	0.00000	-0.00053	-0.00053
2.03039					
A35	2.18063	0.00016	0.00000	0.00156	0.00155
2.18218					
A36	2.07073	-0.00008	0.00000	-0.00110	-0.00110
2.06963					

A37	2.08363	-0.00003	0.00000	0.00135	0.00134	2.08497
A38	2.09553	0.00001	0.00000	0.00046	0.00046	2.09599
A39	2.10396	0.00001	0.00000	-0.00181	-0.00180	2.10216
A40	2.08301	0.00005	0.00000	0.00000	0.00000	2.08301
A41	2.11151	-0.00004	0.00000	0.00013	0.00013	2.11164
A42	2.08866	-0.00001	0.00000	-0.00013	-0.00013	2.08854
A43	2.09485	-0.00004	0.00000	0.00008	0.00008	2.09493
A44	2.09225	0.00007	0.00000	-0.00016	-0.00016	2.09209
A45	2.09609	-0.00004	0.00000	0.00007	0.00007	2.09616
A46	2.09512	0.00005	0.00000	0.00027	0.00027	2.09539
A47	2.08342	-0.00001	0.00000	-0.00019	-0.00019	2.08323
A48	2.10438	-0.00004	0.00000	-0.00008	-0.00008	2.10430
A49	1.88295	0.00003	0.00000	0.00013	0.00013	1.88307
A50	2.28846	-0.00003	0.00000	0.00005	0.00005	2.28851
A51	2.11177	0.00000	0.00000	-0.00017	-0.00017	2.11160
A52	1.88803	0.00001	0.00000	0.00021	0.00021	1.88824
A53	2.26124	0.00000	0.00000	-0.00030	-0.00030	2.26094
A54	2.13370	-0.00001	0.00000	0.00008	0.00008	2.13378
A55	1.90751	0.00005	0.00000	-0.00007	-0.00007	1.90744
A56	2.00262	0.00011	0.00000	-0.00016	-0.00017	2.00246
A57	2.18994	-0.00012	0.00000	0.00078	0.00076	2.19070
A58	2.08885	0.00004	0.00000	-0.00030	-0.00030	2.08855
D1	-0.57155	0.00007	0.00000	0.00345	0.00345	-0.56810
D2	2.84216	0.00016	0.00000	0.00276	0.00276	2.84492
D3	2.59407	0.00010	0.00000	0.00636	0.00636	2.60043
D4	-0.27540	0.00020	0.00000	0.00567	0.00567	-0.26973

This journal is © The Royal Society of Chemistry 2014

D5	-0.02779	0.00002	0.00000	-0.00201	-0.00201	-0.02980
D6	-3.09421	0.00002	0.00000	0.00018	0.00018	-3.09403
D7	3.09129	-0.00002	0.00000	-0.00475	-0.00475	3.08654
D8	0.02487	-0.00002	0.00000	-0.00256	-0.00256	0.02231
D9	-0.05542	0.00002	0.00000	0.00086	0.00086	-0.05456
D10	3.12561	-0.00002	0.00000	-0.00061	-0.00061	3.12500
D11	3.11056	0.00005	0.00000	0.00381	0.00381	3.11437
D12	0.00840	0.00002	0.00000	0.00234	0.00234	0.01074
D13	0.56319	-0.00007	0.00000	-0.00238	-0.00238	0.56081
D14	-2.62515	-0.00009	0.00000	-0.00423	-0.00424	-2.62938
D15	-2.86259	-0.00015	0.00000	-0.00187	-0.00187	-2.86446
D16	0.23226	-0.00018	0.00000	-0.00373	-0.00373	0.22853
D17	-0.35964	0.00016	0.00000	-0.00010	-0.00010	-0.35974
D18	2.84648	-0.00035	0.00000	-0.00576	-0.00576	2.84072
D19	3.06776	0.00023	0.00000	-0.00097	-0.00097	3.06679
D20	-0.00930	-0.00028	0.00000	-0.00663	-0.00663	-0.01593
D21	-3.09415	-0.00001	0.00000	-0.00020	-0.00021	-3.09436
D22	0.63266	-0.00002	0.00000	-0.00034	-0.00034	0.63232
D23	-0.02996	-0.00002	0.00000	-0.00246	-0.00247	-0.03243
D24	-2.58634	-0.00003	0.00000	-0.00260	-0.00260	-2.58894
D25	-0.04204	0.00001	0.00000	0.00100	0.00100	-0.04104
D26	3.11397	0.00000	0.00000	0.00022	0.00022	3.11419
D27	-3.10336	0.00001	0.00000	0.00334	0.00334	-3.10002
D28	0.05266	0.00000	0.00000	0.00255	0.00255	0.05521
D29	-0.64091	0.00007	0.00000	0.00158	0.00158	-0.63933
D30	2.59653	0.00008	0.00000	0.00245	0.00245	2.59898

This journal is © The Royal Society of Chemistry 2014

D31	3.08851	0.00006	0.00000	0.00150	0.00150	3.09001
D32	0.04276	0.00007	0.00000	0.00237	0.00237	0.04513
D33	-0.17322	0.00000	0.00000	-0.00143	-0.00143	-0.17465
D34	2.51358	-0.00002	0.00000	0.00090	0.00090	2.51447
D35	-2.62878	0.00006	0.00000	0.00053	0.00053	-2.62825
D36	0.05802	0.00003	0.00000	0.00286	0.00286	0.06087
D37	-2.63475	0.00000	0.00000	0.00015	0.00015	-2.63460
D38	0.52958	0.00001	0.00000	0.00029	0.00029	0.52988
D39	-0.13294	-0.00002	0.00000	-0.00153	-0.00153	-0.13446
D40	3.03140	-0.00001	0.00000	-0.00139	-0.00139	3.03001
D41	0.03433	-0.00003	0.00000	-0.00328	-0.00328	0.03106
D42	-3.10435	-0.00005	0.00000	-0.00380	-0.00380	-3.10816
D43	2.75463	-0.00002	0.00000	-0.00079	-0.00079	2.75384
D44	-0.38406	-0.00003	0.00000	-0.00131	-0.00132	-0.38537
D45	3.11561	0.00001	0.00000	0.00010	0.00010	3.11571
D46	-0.02497	-0.00001	0.00000	-0.00058	-0.00057	-0.02554
D47	0.01290	-0.00003	0.00000	-0.00135	-0.00135	0.01155
D48	-3.12768	-0.00004	0.00000	-0.00202	-0.00202	-3.12970
D49	-3.13284	0.00001	0.00000	-0.00001	-0.00001	-3.13285
D50	0.00792	0.00000	0.00000	-0.00104	-0.00104	0.00688
D51	0.00977	-0.00001	0.00000	-0.00069	-0.00069	0.00908
D52	-3.13266	-0.00002	0.00000	-0.00172	-0.00172	-3.13438
D53	0.02560	0.00001	0.00000	0.00082	0.00082	0.02642
D54	-3.13060	0.00001	0.00000	0.00161	0.00161	-3.12899
D55	-3.11683	-0.00001	0.00000	-0.00021	-0.00021	-3.11704
D56	0.01015	0.00000	0.00000	0.00058	0.00058	0.01073

This journal is © The Royal Society of Chemistry 2014

D57	0.03988	0.00004	0.00000	-0.00010	-0.00010	0.03978
D58	-3.05805	0.00005	0.00000	0.00156	0.00156	-3.05649
D59	3.08783	0.00004	0.00000	-0.00102	-0.00102	3.08681
D60	-0.01009	0.00005	0.00000	0.00063	0.00063	-0.00946
D61	3.08076	-0.00004	0.00000	-0.00131	-0.00131	3.07945
D62	-0.08534	-0.00002	0.00000	-0.00101	-0.00101	-0.08635
D63	0.03820	-0.00003	0.00000	-0.00041	-0.00041	0.03779
D64	-3.12790	-0.00001	0.00000	-0.00011	-0.00011	-3.12801
D65	0.03522	-0.00006	0.00000	0.00182	0.00182	0.03704
D66	-3.11907	-0.00001	0.00000	0.00151	0.00151	-3.11756
D67	3.12909	-0.00008	0.00000	-0.00006	-0.00006	3.12903
D68	-0.02521	-0.00003	0.00000	-0.00037	-0.00037	-0.02558
D69	-3.10922	-0.00001	0.00000	-0.00019	-0.00019	-3.10940
D70	0.03308	0.00000	0.00000	-0.00011	-0.00011	0.03297
D71	0.01952	0.00004	0.00000	-0.00047	-0.00047	0.01905
D72	-3.12137	0.00005	0.00000	-0.00039	-0.00039	-3.12176
D73	3.13884	0.00000	0.00000	0.00019	0.00019	3.13903
D74	-0.00483	0.00002	0.00000	0.00034	0.00035	-0.00449
D75	-0.00205	0.00001	0.00000	0.00027	0.00027	-0.00178
D76	3.13746	0.00003	0.00000	0.00042	0.00043	3.13789
D77	-0.03081	-0.00001	0.00000	-0.00008	-0.00008	-0.03089
D78	3.13559	-0.00003	0.00000	-0.00038	-0.00038	3.13521
D79	3.10870	0.00001	0.00000	0.00008	0.00008	3.10878
D80	-0.00809	-0.00001	0.00000	-0.00022	-0.00022	-0.00831
D81	-0.12090	0.00002	0.00000	0.00231	0.00231	-0.11858
D82	3.01814	0.00003	0.00000	0.00278	0.00278	3.02092

```
   D83        0.15721   0.00001   0.00000  -0.00052  -0.00052
0.15669
   D84       -3.00511  -0.00001   0.00000  -0.00066  -0.00066  -
3.00577
         Item               Value     Threshold  Converged?
 Maximum Force            0.000411     0.000450     YES
 RMS     Force            0.000094     0.000300     YES
 Maximum Displacement     0.028445     0.001800     NO
 RMS     Displacement     0.004749     0.001200     NO
 Predicted change in Energy=-7.838553D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.555687    0.522979    1.163951
    2          6             0        0.604789    1.085336    0.492626
    3          6             0       -0.741199   -0.883770    1.059720
    4          6             0        0.225538   -1.603903    0.263016
    5          1             0        0.063166   -2.673731    0.142126
    6          6             0       -0.204271   -0.963526   -1.635718
    7          1             0        0.490867   -1.646003   -2.110793
    8          6             0       -0.096865    0.442713   -1.721306
    9          1             0        0.737439    1.003156   -2.119391
   10          6             0       -1.516268    1.280698    1.878207
   11          1             0       -1.394176    2.351536    1.999597
   12          6             0       -2.601469    0.654269    2.469227
   13          1             0       -3.317223    1.244872    3.034356
   14          6             0       -2.786449   -0.737200    2.346081
   15          1             0       -3.646961   -1.212214    2.808613
   16          6             0       -1.873424   -1.497074    1.634471
   17          1             0       -2.012283   -2.569124    1.523160
   18          6             0        1.597380   -1.143174    0.318802
   19          6             0        1.802398    0.262094    0.411746
   20          6             0        3.128211    0.758157    0.362916
   21          1             0        3.299634    1.824482    0.420517
   22          6             0        4.196261   -0.120812    0.257710
   23          1             0        5.209908    0.271011    0.251600
   24          6             0        3.985206   -1.509918    0.158069
   25          1             0        4.833251   -2.184213    0.073934
   26          6             0        2.694360   -2.014566    0.169882
   27          1             0        2.518037   -3.084700    0.087662
   28          6             0       -1.462213    0.992924   -1.783251
   29          6             0       -1.662418   -1.277132   -1.733138
   30          8             0       -2.366080   -0.082014   -1.692765
   31          8             0       -2.212698   -2.343674   -1.810142
   32          8             0       -1.855034    2.125208   -1.892227
   33          6             0        0.630270    2.556228    0.248012
```

34	1	0	-0.358637	3.044812	0.268942
35	8	0	1.623104	3.213204	-0.021339

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.453832	0.000000			
3	C	1.422752	2.451665	0.000000		
4	C	2.438365	2.725539	1.444959	0.000000	
5	H	3.412632	3.814026	2.166320	1.088812	0.000000
6	C	3.189253	3.063048	2.749552	2.049392	2.481340
7	H	4.064937	3.775048	3.485848	2.388963	2.512926
8	C	2.922613	2.409726	3.147829	2.868818	3.634585
9	H	3.561331	2.616674	3.981659	3.568566	4.369050
10	C	1.416691	2.541040	2.440404	3.736797	4.598488
11	H	2.178300	2.805367	3.431757	4.613533	5.552239
12	C	2.430268	3.791156	2.795153	4.237767	4.857084
13	H	3.412569	4.676326	3.881521	5.324190	5.928530
14	C	2.821662	4.272871	2.420589	3.763295	4.089972
15	H	3.907913	5.359097	3.407339	4.650778	4.797002
16	C	2.457323	3.756887	1.410112	2.509570	2.713300
17	H	3.436831	4.611524	2.161215	2.743621	2.495132
18	C	2.850622	2.445753	2.466820	1.448218	2.174312
19	C	2.488863	1.455520	2.864046	2.447560	3.422965
20	C	3.777311	2.547848	4.260727	3.743637	4.606637
21	H	4.136436	2.795303	4.906275	4.607461	5.548526
22	C	4.880241	3.795873	5.060024	4.238659	4.859345
23	H	5.842770	4.682770	6.115738	5.325352	5.930636
24	C	5.075843	4.274867	4.852210	3.762307	4.091102
25	H	6.128433	5.361450	5.808392	4.647960	4.795622
26	C	4.241476	3.752315	3.724725	2.504477	2.712647
27	H	4.860199	4.605835	4.051124	2.734787	2.489630
28	C	3.119076	3.075818	3.482000	3.712038	4.413413
29	C	3.585858	3.959231	2.967057	2.766909	2.905983
30	O	3.435748	3.868424	3.295334	3.585765	3.998131
31	O	4.450687	4.999909	3.540161	3.284851	3.016595
32	O	3.687230	3.580445	4.359882	4.783317	5.554088
33	C	2.525775	1.491311	3.791225	4.179800	5.261681
34	H	2.683190	2.194942	4.025598	4.685280	5.735480
35	O	3.659146	2.414320	4.852196	5.023800	6.092300

		6	7	8	9	10
6	C	0.000000				
7	H	1.083830	0.000000			
8	C	1.412929	2.204510	0.000000		
9	H	2.233516	2.660624	1.081033	0.000000	
10	C	4.370989	5.339128	3.958966	4.597500	0.000000
11	H	5.061722	6.035646	4.378555	4.829904	1.084591
12	C	5.021393	5.985848	4.886549	5.685546	1.385416
13	H	6.031342	7.023622	5.799180	6.561998	2.140422
14	C	4.751167	5.606286	5.016940	5.948702	2.429851
15	H	5.627259	6.442853	5.988500	6.958165	3.408829
16	C	3.710106	4.431598	4.263822	5.211453	2.811224

This journal is © The Royal Society of Chemistry 2014

17	H	3.978111	4.508162	4.823541	5.795717	3.897848
18	C	2.664276	2.716641	3.089910	3.360211	4.242842
19	C	3.117847	3.424055	2.861771	2.844286	3.768502
20	C	4.250196	4.342212	3.852869	3.455093	4.913283
21	H	4.927315	5.132345	4.246516	3.700075	5.060975
22	C	4.864146	4.654672	4.760777	4.344809	6.101085
23	H	5.865098	5.614730	5.664245	5.114745	6.993337
24	C	4.589981	4.168532	4.899808	4.695781	6.404110
25	H	5.457986	4.890706	5.867680	5.634330	7.455026
26	C	3.573085	3.192601	4.172020	4.263445	5.613068
27	H	3.857509	3.318504	4.748970	4.975156	6.207928
28	C	2.330640	3.299355	1.473345	2.225210	3.673147
29	C	1.494668	2.217053	2.325717	3.332899	4.427828
30	O	2.335324	3.283741	2.329268	3.315333	3.915483
31	O	2.443157	2.808273	3.499799	4.472160	5.217758
32	O	3.511565	4.446690	2.439500	2.833993	3.878676
33	C	4.078427	4.821011	2.978907	2.833393	2.981969
34	H	4.440533	5.328090	3.286416	3.327743	2.653666
35	O	4.836382	5.409221	3.677472	3.173411	4.147108

		11	12	13	14	15
11	H	0.000000				
12	C	2.135140	0.000000			
13	H	2.448172	1.086502	0.000000		
14	C	3.405696	1.409103	2.164267	0.000000	
15	H	4.293002	2.166102	2.489369	1.086304	0.000000
16	C	3.895484	2.419740	3.400367	1.384705	2.145970
17	H	4.982163	3.410638	4.305014	2.152319	2.483097
18	C	4.897702	5.048313	6.101666	4.846920	5.805777
19	C	4.135835	4.876584	5.835620	5.079149	6.133032
20	C	5.066515	6.105454	6.994077	6.415001	7.467715
21	H	4.980274	6.355283	7.137990	6.878256	7.948566
22	C	6.356073	7.190319	8.125719	7.314333	8.319520
23	H	7.141288	8.129106	9.022422	8.327368	9.337152
24	C	6.873122	7.308176	8.317894	7.158198	8.084800
25	H	7.941162	8.310805	9.324857	8.081852	8.963106
26	C	6.255145	6.360462	7.414060	6.033803	6.915131
27	H	6.965169	6.772081	7.840820	6.224852	6.994068
28	C	4.020000	4.415446	5.168547	4.668866	5.542651
29	C	5.212725	4.719321	5.641621	4.265559	4.956827
30	O	4.527727	4.233167	5.001098	4.113181	4.814605
31	O	6.101565	5.239447	6.129176	4.492676	4.966912
32	O	3.925546	4.662951	5.213849	5.198477	6.037159
33	C	2.684833	4.358369	5.006603	5.188692	6.249203
34	H	2.132637	3.947942	4.431764	4.950999	5.948553
35	O	3.732376	5.531552	6.133387	6.376089	7.440869

		16	17	18	19	20
16	C	0.000000				
17	H	1.086722	0.000000			
18	C	3.728635	4.063679	0.000000		
19	C	4.254574	4.878814	1.423182	0.000000	
20	C	5.631987	6.232307	2.441403	1.416419	0.000000
21	H	6.266334	6.981121	3.422717	2.163989	1.081551

This journal is © The Royal Society of Chemistry 2014

22	C	6.374218	6.792762	2.793410	2.429182	1.387222
23	H	7.430481	7.864049	3.880050	3.411282	2.140832
24	C	6.041811	6.241415	2.421167	2.822946	2.433221
25	H	6.920039	7.007835	3.408017	3.909553	3.412948
26	C	4.824674	4.928629	1.408853	2.457086	2.813091
27	H	4.919158	4.780196	2.161148	3.437761	3.900721
28	C	4.248531	4.891127	4.282832	4.001226	5.072784
29	C	3.381374	3.520671	3.854177	4.355995	5.611236
30	O	3.649056	4.080817	4.569626	4.682263	5.926124
31	O	3.563313	3.346924	4.526622	5.277103	6.547431
32	O	5.055578	5.807440	5.243103	4.707047	5.638016
33	C	4.961856	5.905788	3.824381	2.581424	3.079932
34	H	4.978753	5.985306	4.622523	3.526186	4.170820
35	O	6.095419	7.002630	4.369712	2.988103	2.905212

		21	22	23	24	25
21	H	0.000000				
22	C	2.148165	0.000000			
23	H	2.467985	1.086757	0.000000		
24	C	3.414251	1.408577	2.163412	0.000000	
25	H	4.306012	2.167292	2.490293	1.086708	0.000000
26	C	3.894543	2.418621	3.399782	1.386034	2.147752
27	H	4.982143	3.410277	4.305095	2.153481	2.484207
28	C	5.312557	6.117537	7.012772	6.301374	7.292201
29	C	6.235398	6.294813	7.318797	5.960411	6.803088
30	O	6.340426	6.846180	7.829481	6.767816	7.705247
31	O	7.261898	7.091678	8.135259	6.556144	7.295243
32	O	5.657722	6.803308	7.612321	7.178179	8.195734
33	C	2.773214	4.459028	5.118136	5.272308	6.337755
34	H	3.859421	5.546927	6.221171	6.294985	7.371325
35	O	2.221382	4.220743	4.647167	5.283900	6.280624

		26	27	28	29	30
26	C	0.000000				
27	H	1.087675	0.000000			
28	C	5.489702	5.997476	0.000000		
29	C	4.811113	4.904978	2.279419	0.000000	
30	O	5.728199	6.003386	1.407358	1.387472	0.000000
31	O	5.301701	5.150790	3.420064	1.202601	2.269891
32	O	6.487450	7.084267	1.203432	3.411499	2.274375
33	C	5.015849	5.950584	3.308841	4.886309	4.439037
34	H	5.909985	6.773407	3.104773	4.938357	4.201805
35	O	5.339825	6.362105	4.189648	5.821342	5.437436

		31	32	33	34	35
31	O	0.000000				
32	O	4.483923	0.000000			
33	C	6.027230	3.308041	0.000000		
34	H	6.065963	2.784874	1.103218	0.000000	
35	O	6.985133	4.096510	1.220609	2.009954	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1

This journal is © The Royal Society of Chemistry 2014

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.520678	0.684831	1.084766
2	6	0	0.627997	1.130775	0.313204
3	6	0	-0.723963	-0.719829	1.183911
4	6	0	0.213992	-1.558376	0.473287
5	1	0	0.037032	-2.632150	0.508003
6	6	0	-0.257964	-1.184672	-1.485696
7	1	0	0.417239	-1.936928	-1.876720
8	6	0	-0.137679	0.193964	-1.770760
9	1	0	0.692012	0.681018	-2.263733
10	6	0	-1.454211	1.548932	1.708352
11	1	0	-1.317492	2.624353	1.674962
12	6	0	-2.530411	1.027212	2.407624
13	1	0	-3.224878	1.701442	2.901199
14	6	0	-2.733490	-0.364982	2.485886
15	1	0	-3.586790	-0.758042	3.031267
16	6	0	-1.847449	-1.230165	1.866371
17	1	0	-2.000679	-2.305132	1.910313
18	6	0	1.591700	-1.114043	0.430582
19	6	0	1.814175	0.287286	0.320003
20	6	0	3.143541	0.752579	0.169896
21	1	0	3.327868	1.813876	0.072813
22	6	0	4.198980	-0.147638	0.163585
23	1	0	5.216287	0.224915	0.077958
24	6	0	3.970471	-1.533822	0.265408
25	1	0	4.808742	-2.225309	0.256481
26	6	0	2.675007	-2.013308	0.379240
27	1	0	2.485101	-3.081760	0.452610
28	6	0	-1.498171	0.749509	-1.876477
29	6	0	-1.721438	-1.487961	-1.502806
30	8	0	-2.410910	-0.289062	-1.613923
31	8	0	-2.284980	-2.546776	-1.415748
32	8	0	-1.881472	1.860801	-2.134084
33	6	0	0.662963	2.552276	-0.136373
34	1	0	-0.319752	3.053055	-0.160486
35	8	0	1.655498	3.150693	-0.519332

Rotational constants (GHZ): 0.3891754 0.2596010 0.2421591

Standard basis: 6-31+G(d) (6D, 7F)

There are 461 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

461 basis functions, 784 primitive gaussians, 461 cartesian basis functions

79 alpha electrons 79 beta electrons

```
       nuclear repulsion energy      1907.0103846341 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
```

This journal is © The Royal Society of Chemistry 2014

```
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1032.13801478     A.U. after   14 cycles
            Convg  =    0.5602D-08             -V/T =  2.0093
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000007429    0.000056976   -0.000036773
    2          6          -0.000054697    0.000008934   -0.000172864
    3          6           0.000014928   -0.000008305   -0.000001189
    4          6           0.000017319    0.000010777    0.000070257
    5          1          -0.000001781   -0.000009992    0.000011476
    6          6          -0.000042029   -0.000030492   -0.000108779
    7          1           0.000012801   -0.000008994   -0.000001238
    8          6           0.000041846    0.000036123    0.000138169
    9          1           0.000013076    0.000013971    0.000009472
   10          6          -0.000009028   -0.000008672    0.000015367
   11          1           0.000013926   -0.000008301    0.000037700
   12          6          -0.000002022   -0.000006196    0.000001014
   13          1           0.000000306   -0.000003754    0.000001742
   14          6          -0.000000277    0.000001408   -0.000000565
   15          1           0.000000751   -0.000003456   -0.000001364
   16          6           0.000007948    0.000004881   -0.000013324
   17          1           0.000001303   -0.000001708   -0.000003199
   18          6          -0.000006810   -0.000006411    0.000008472
   19          6          -0.000018614   -0.000016605    0.000033311
   20          6           0.000059691   -0.000016897    0.000011041
   21          1           0.000044010   -0.000038724   -0.000033884
   22          6          -0.000001918   -0.000002481    0.000003389
   23          1           0.000000907   -0.000001796    0.000000245
   24          6          -0.000013400    0.000012181   -0.000002227
   25          1           0.000000266    0.000002265   -0.000001931
   26          6           0.000016953    0.000005243   -0.000002830
   27          1           0.000004507    0.000000403   -0.000001568
   28          6          -0.000014392    0.000024755   -0.000018433
   29          6           0.000011737   -0.000011597    0.000010661
   30          8          -0.000008849   -0.000006733    0.000006932
   31          8          -0.000002821   -0.000003419   -0.000004991
   32          8           0.000001340   -0.000000491    0.000009370
   33          6          -0.000001838   -0.000011252   -0.000016138
   34          1           0.000002843   -0.000006363   -0.000034687
   35          8          -0.000080553    0.000034721    0.000087367
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000172864 RMS     0.000032846
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000104429 RMS     0.000018881
 Search for a saddle point.
 Step number   6 out of a maximum of 202
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Update second derivatives using D2CorX and points  4  5  6
     Eigenvalues ---   -0.01884   0.00022   0.00626   0.00786
0.00862
     Eigenvalues ---    0.01083   0.01262   0.01435   0.01484
0.01531
     Eigenvalues ---    0.01629   0.01693   0.01774   0.01851
0.01918
     Eigenvalues ---    0.01983   0.02111   0.02173   0.02191
0.02232
     Eigenvalues ---    0.02360   0.02427   0.02449   0.02522
0.02681
     Eigenvalues ---    0.02724   0.02746   0.02751   0.03185
0.03524
     Eigenvalues ---    0.04126   0.05546   0.07030   0.07471
0.07684
     Eigenvalues ---    0.08788   0.10191   0.11049   0.11179
0.11224
     Eigenvalues ---    0.11854   0.12288   0.12499   0.12527
0.12660
     Eigenvalues ---    0.12835   0.13904   0.14278   0.14661
0.16375
     Eigenvalues ---    0.17650   0.18504   0.19087   0.19175
0.19334
     Eigenvalues ---    0.19418   0.20109   0.20421   0.20904
0.21163
     Eigenvalues ---    0.23350   0.23905   0.24401   0.25100
0.26055
     Eigenvalues ---    0.27641   0.27928   0.29110   0.30147
0.30306
     Eigenvalues ---    0.31236   0.33089   0.33997   0.34040
0.35018
     Eigenvalues ---    0.35278   0.35919   0.36086   0.36133
0.36202
     Eigenvalues ---    0.36237   0.36329   0.36535   0.37432
0.37823
     Eigenvalues ---    0.38853   0.39861   0.40318   0.41112
0.42459
     Eigenvalues ---    0.44484   0.46388   0.47305   0.47638
0.50257
     Eigenvalues ---    0.50619   0.79395   0.89039
0.902561000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
          1            -0.04248   0.02345   0.15563   0.01777
0.36824
                           R6        R7        R8        R9        R10
          1             0.10085  -0.04331  -0.02059  -0.06098
0.19382
                           R11       R12       R13       R14       R15
          1             0.01913  -0.00704   0.44415   0.18355  -
0.05904
                           R16       R17       R18       R19       R20
          1             0.29250  -0.00750  -0.09421   0.18585  -
0.01333
                           R21       R22       R23       R24       R25
          1            -0.02845  -0.00712   0.15692  -0.00584  -
0.04119
                           R26       R27       R28       R29       R30
```

This journal is © The Royal Society of Chemistry 2014

1	0.06055	-0.00141	-0.01352	0.00008	0.01442

	R31	R32	R33	R34	R35
1	-0.00023	-0.01604	-0.00025	0.02092	0.01821

	R36	R37	R38	R39	R40
1	0.01739	-0.00150	-0.01215	-0.04764	0.00008

	R41	R42	R43	R44	R45
1	0.01320	-0.00013	-0.01533	-0.00014	0.00236

	R46	R47	R48	R49	R50
1	0.00082	-0.00160	0.00268	-0.00131	0.00508

	A1	A2	A3	A4	A5
1	0.02097	-0.00754	-0.01334	0.03192	-0.00172

	A6	A7	A8	A9	A10
1	0.00550	0.01914	-0.00134	-0.01664	0.03325

	A11	A12	A13	A14	A15
1	0.05668	0.02992	0.06223	0.04264	0.02270

	A16	A17	A18	A19	A20
1	0.04694	0.00713	0.01637	-0.00362	0.00685

	A21	A22	A23	A24	A25
1	-0.00330	-0.00134	0.00489	-0.00356	-0.00133

	A26	A27	A28	A29	A30
1	-0.00136	0.00270	0.00416	-0.00661	0.00237

	A31	A32	A33	A34	A35
1	0.01941	-0.01770	-0.00071	0.02140	-0.00804

	A36	A37	A38	A39	A40
1	-0.01324	-0.00351	0.00689	-0.00339	-0.00104

	A41	A42	A43	A44	A45
1	0.00436	-0.00332	-0.00116	-0.00144	0.00259

	A46	A47	A48	A49	A50
1	0.00414	-0.00627	0.00203	-0.00245	0.00206

	A51	A52	A53	A54	A55
1	0.00038	-0.00669	0.00415	0.00263	-0.01362

	A56	A57	A58	D1	D2
1	-0.00036	0.00839	-0.00822	0.13183	-0.00724

	D3	D4	D5	D6	D7

```
          1              0.12809  -0.01099   0.02025   0.00470
0.02381
                           D8        D9        D10       D11       D12
          1              0.00826  -0.00344  -0.00132  -0.00773  -
0.00561
                           D13       D14       D15       D16       D17
          1             -0.13539  -0.13274   0.00902   0.01167
0.10312
                           D18       D19       D20       D21       D22
          1              0.10719  -0.04713  -0.04306   0.05272  -
0.15936
                           D23       D24       D25       D26       D27
          1              0.06954  -0.14255  -0.00506   0.00101  -
0.02336
                           D28       D29       D30       D31       D32
          1             -0.01729   0.15552   0.14368  -0.05871  -
0.07056
                           D33       D34       D35       D36       D37
          1              0.01273   0.17788  -0.17165  -0.00650  -
0.15141
                           D38       D39       D40       D41       D42
          1             -0.15606   0.03009   0.02545  -0.01849  -
0.01571
                           D43       D44       D45       D46       D47
          1              0.14401   0.14680  -0.00142  -0.00063
0.00068
                           D48       D49       D50       D51       D52
          1              0.00147   0.00019   0.00405   0.00098
0.00484
                           D53       D54       D55       D56       D57
          1             -0.00115  -0.00737   0.00271  -0.00351  -
0.01232
                           D58       D59       D60       D61       D62
          1             -0.01486  -0.00177  -0.00431   0.01523
0.01055
                           D63       D64       D65       D66       D67
          1              0.00196  -0.00273   0.00098  -0.00038
0.00457
                           D68       D69       D70       D71       D72
          1              0.00321   0.00213   0.00057   0.00075  -
0.00080
                           D73       D74       D75       D76       D77
          1              0.00087  -0.00288  -0.00069  -0.00444
0.00162
                           D78       D79       D80       D81       D82
          1              0.00648  -0.00214   0.00272   0.03975
0.03731
                           D83       D84
          1             -0.04573  -0.04146
 RFO step:  Lambda0=2.127846071D-08 Lambda=-3.45336544D-05.
 Linear search not attempted -- option 19 set.
 Maximum step size (   0.300) exceeded in Quadratic search.
```

This journal is © The Royal Society of Chemistry 2014

```
    -- Step size scaled by   0.841
 Iteration  1 RMS(Cart)=  0.02833601 RMS(Int)=  0.00188553
 Iteration  2 RMS(Cart)=  0.00240625 RMS(Int)=  0.00034366
 Iteration  3 RMS(Cart)=  0.00000998 RMS(Int)=  0.00034359
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00034359
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.74735   0.00000   0.00000   0.00029   0.00026
2.74761
    R2        2.68861   0.00000   0.00000  -0.00049  -0.00032
2.68829
    R3        5.52294  -0.00003   0.00000   0.01789   0.01793
5.54087
    R4        2.67716   0.00002   0.00000   0.00029   0.00026
2.67742
    R5        4.55372  -0.00004   0.00000   0.03790   0.03826
4.59199
    R6        4.94480  -0.00004   0.00000   0.05943   0.05981
5.00461
    R7        2.75053   0.00004   0.00000  -0.00176  -0.00299
2.74755
    R8        2.81817  -0.00004   0.00000   0.00125   0.00078
2.81895
    R9        2.73058  -0.00002   0.00000   0.00070   0.00094
2.73151
   R10        5.19590   0.00001   0.00000  -0.00612  -0.00620
5.18970
   R11        2.66473  -0.00001   0.00000  -0.00059  -0.00060
2.66412
   R12        2.05756   0.00001   0.00000   0.00026   0.00033
2.05788
   R13        3.87279   0.00001   0.00000  -0.00926  -0.00935
3.86344
   R14        4.51449   0.00003   0.00000  -0.00550  -0.00555
4.50894
   R15        2.73674  -0.00001   0.00000   0.00120   0.00140
2.73814
   R16        4.68905   0.00000   0.00000  -0.00572  -0.00584
4.68321
   R17        2.04814  -0.00001   0.00000   0.00031   0.00031
2.04845
   R18        2.67005   0.00005   0.00000   0.00229   0.00215
2.67220
   R19        5.03475   0.00001   0.00000  -0.00098  -0.00088
5.03387
   R20        2.82451   0.00000   0.00000   0.00086   0.00087
2.82538
   R21        5.13371   0.00001   0.00000   0.00281   0.00291
5.13662
   R22        2.04286   0.00003   0.00000   0.00073   0.00063
2.04348
```

This journal is © The Royal Society of Chemistry 2014

R23	5.40796	-0.00001	0.00000	0.02977	0.02949
5.43745					
R24	2.78422	0.00002	0.00000	-0.00125	-0.00127
2.78295					
R25	5.37492	-0.00001	0.00000	0.05096	0.05091
5.42583					
R26	5.35434	0.00001	0.00000	0.07656	0.07609
5.43043					
R27	2.04958	0.00000	0.00000	0.00025	0.00025
2.04983					
R28	2.61806	0.00000	0.00000	0.00013	0.00014
2.61820					
R29	2.05319	0.00000	0.00000	-0.00001	-0.00001
2.05318					
R30	2.66282	-0.00001	0.00000	-0.00006	-0.00003
2.66279					
R31	2.05282	0.00000	0.00000	-0.00001	-0.00001
2.05280					
R32	2.61671	0.00000	0.00000	0.00036	0.00038
2.61709					
R33	2.05361	0.00000	0.00000	-0.00003	-0.00003
2.05357					
R34	2.68942	0.00000	0.00000	0.00032	-0.00007
2.68935					
R35	2.66235	0.00001	0.00000	-0.00004	-0.00002
2.66232					
R36	2.67664	0.00004	0.00000	-0.00027	-0.00108
2.67557					
R37	2.04384	0.00000	0.00000	0.00070	0.00121
2.04505					
R38	2.62147	-0.00001	0.00000	0.00022	0.00021
2.62168					
R39	4.19780	0.00008	0.00000	-0.00701	-0.00599
4.19182					
R40	2.05367	0.00000	0.00000	0.00005	0.00005
2.05372					
R41	2.66183	-0.00001	0.00000	0.00021	0.00052
2.66234					
R42	2.05358	0.00000	0.00000	0.00001	0.00001
2.05359					
R43	2.61923	-0.00001	0.00000	0.00044	0.00076
2.61999					
R44	2.05541	0.00000	0.00000	0.00007	0.00007
2.05548					
R45	2.65952	0.00002	0.00000	0.00083	0.00083
2.66036					
R46	2.27416	0.00000	0.00000	0.00042	0.00042
2.27458					
R47	2.62194	0.00001	0.00000	0.00022	0.00023
2.62218					
R48	2.27259	0.00001	0.00000	0.00006	0.00006
2.27265					

This journal is © The Royal Society of Chemistry 2014

R49	2.08478	-0.00001	0.00000	0.00021	0.00021
2.08499					
R50	2.30662	-0.00005	0.00000	0.00036	0.00060
2.30722					
A1	2.04060	-0.00002	0.00000	0.00170	0.00147
2.04207					
A2	2.17384	0.00003	0.00000	-0.00149	-0.00133
2.17251					
A3	2.06845	-0.00001	0.00000	-0.00001	0.00003
2.06847					
A4	2.05292	0.00000	0.00000	0.00100	0.00121
2.05412					
A5	2.06110	-0.00004	0.00000	-0.00894	-0.00729
2.05381					
A6	2.13493	0.00003	0.00000	0.00919	0.00721
2.14214					
A7	2.03301	0.00002	0.00000	-0.00044	-0.00046
2.03255					
A8	2.10003	0.00000	0.00000	0.00030	0.00026
2.10029					
A9	2.14739	-0.00002	0.00000	0.00012	0.00019
2.14758					
A10	2.03883	-0.00001	0.00000	-0.00154	-0.00150
2.03733					
A11	2.04201	0.00001	0.00000	0.00021	0.00019
2.04219					
A12	2.04668	0.00000	0.00000	-0.00159	-0.00156
2.04513					
A13	2.15484	0.00001	0.00000	-0.00207	-0.00210
2.15274					
A14	2.05444	0.00000	0.00000	-0.00073	-0.00069
2.05376					
A15	1.85358	0.00001	0.00000	-0.00127	-0.00128
1.85231					
A16	2.21049	0.00001	0.00000	-0.00454	-0.00476
2.20573					
A17	1.87945	-0.00001	0.00000	0.00086	0.00092
1.88037					
A18	2.10146	0.00000	0.00000	-0.00008	0.00002
2.10148					
A19	2.10385	0.00000	0.00000	-0.00014	-0.00012
2.10373					
A20	2.09943	0.00000	0.00000	-0.00011	-0.00016
2.09928					
A21	2.07928	-0.00001	0.00000	0.00010	0.00012
2.07940					
A22	2.08532	0.00000	0.00000	0.00000	-0.00001
2.08531					
A23	2.10836	0.00000	0.00000	-0.00008	-0.00007
2.10830					
A24	2.08950	0.00000	0.00000	0.00008	0.00007
2.08957					

This journal is © The Royal Society of Chemistry 2014

A25	2.09276	0.00000	0.00000	-0.00001	-0.00002
2.09273					
A26	2.09468	0.00000	0.00000	0.00006	0.00009
2.09477					
A27	2.09574	0.00000	0.00000	-0.00005	-0.00007
2.09568					
A28	2.09464	0.00001	0.00000	-0.00015	-0.00017
2.09447					
A29	2.08278	0.00000	0.00000	0.00006	0.00007
2.08285					
A30	2.10568	0.00000	0.00000	0.00008	0.00009
2.10577					
A31	2.04104	0.00000	0.00000	0.00173	0.00144
2.04248					
A32	2.13735	0.00000	0.00000	-0.00183	-0.00112
2.13623					
A33	2.10071	0.00000	0.00000	-0.00010	-0.00052
2.10019					
A34	2.03039	-0.00001	0.00000	-0.00041	0.00009
2.03048					
A35	2.18218	0.00002	0.00000	-0.00012	-0.00155
2.18063					
A36	2.06963	-0.00001	0.00000	0.00012	0.00101
2.07064					
A37	2.08497	-0.00002	0.00000	-0.00100	-0.00174
2.08323					
A38	2.09599	0.00000	0.00000	-0.00018	-0.00045
2.09554					
A39	2.10216	0.00001	0.00000	0.00115	0.00214
2.10430					
A40	2.08301	0.00001	0.00000	-0.00041	-0.00031
2.08270					
A41	2.11164	0.00000	0.00000	0.00046	0.00026
2.11190					
A42	2.08854	0.00000	0.00000	-0.00005	0.00005
2.08859					
A43	2.09493	0.00000	0.00000	0.00046	0.00038
2.09532					
A44	2.09209	0.00001	0.00000	-0.00061	-0.00047
2.09162					
A45	2.09616	0.00000	0.00000	0.00016	0.00009
2.09625					
A46	2.09539	0.00001	0.00000	0.00034	0.00019
2.09558					
A47	2.08323	0.00000	0.00000	-0.00031	-0.00024
2.08299					
A48	2.10430	-0.00001	0.00000	0.00001	0.00008
2.10438					
A49	1.88307	0.00000	0.00000	-0.00012	-0.00015
1.88292					
A50	2.28851	0.00000	0.00000	0.00012	0.00014
2.28865					

This journal is © The Royal Society of Chemistry 2014

A51	2.11160	0.00000	0.00000	0.00000	0.00002	2.11161
A52	1.88824	0.00000	0.00000	0.00036	0.00036	1.88860
A53	2.26094	0.00000	0.00000	-0.00040	-0.00040	2.26054
A54	2.13378	0.00000	0.00000	0.00005	0.00006	2.13384
A55	1.90744	0.00001	0.00000	0.00026	0.00025	1.90769
A56	2.00246	0.00001	0.00000	-0.00826	-0.00750	1.99496
A57	2.19070	-0.00001	0.00000	0.00672	0.00520	2.19590
A58	2.08855	0.00000	0.00000	0.00148	0.00224	2.09079
D1	-0.56810	0.00000	0.00000	0.00448	0.00461	-0.56350
D2	2.84492	0.00002	0.00000	-0.00183	-0.00095	2.84397
D3	2.60043	-0.00003	0.00000	-0.00428	-0.00435	2.59608
D4	-0.26973	0.00000	0.00000	-0.01059	-0.00991	-0.27964
D5	-0.02980	0.00001	0.00000	-0.00325	-0.00327	-0.03307
D6	-3.09403	0.00000	0.00000	-0.00304	-0.00315	-3.09718
D7	3.08654	0.00003	0.00000	0.00493	0.00511	3.09165
D8	0.02231	0.00003	0.00000	0.00514	0.00523	0.02754
D9	-0.05456	-0.00001	0.00000	-0.00121	-0.00109	-0.05565
D10	3.12500	0.00000	0.00000	0.00341	0.00350	3.12850
D11	3.11437	-0.00003	0.00000	-0.01012	-0.01020	3.10417
D12	0.01074	-0.00002	0.00000	-0.00550	-0.00560	0.00514
D13	0.56081	0.00000	0.00000	-0.00139	-0.00142	0.55939
D14	-2.62938	-0.00001	0.00000	-0.01130	-0.01136	-2.64074
D15	-2.86446	-0.00004	0.00000	0.00213	0.00198	-2.86248
D16	0.22853	-0.00005	0.00000	-0.00779	-0.00796	0.22057
D17	-0.35974	-0.00005	0.00000	-0.13284	-0.13305	-0.49279
D18	2.84072	-0.00010	0.00000	-0.13167	-0.13189	2.70883

This journal is © The Royal Society of Chemistry 2014

D19	3.06679	-0.00002	0.00000	-0.13792	-0.13775	2.92904
D20	-0.01593	-0.00007	0.00000	-0.13676	-0.13659	-0.15253
D21	-3.09436	-0.00001	0.00000	-0.00763	-0.00771	-3.10207
D22	0.63232	0.00000	0.00000	-0.00217	-0.00238	0.62994
D23	-0.03243	0.00000	0.00000	-0.00784	-0.00783	-0.04026
D24	-2.58894	0.00001	0.00000	-0.00238	-0.00249	-2.59143
D25	-0.04104	-0.00001	0.00000	-0.00153	-0.00155	-0.04259
D26	3.11419	0.00000	0.00000	-0.00098	-0.00097	3.11321
D27	-3.10002	-0.00002	0.00000	-0.00128	-0.00140	-3.10142
D28	0.05521	-0.00002	0.00000	-0.00073	-0.00082	0.05438
D29	-0.63933	0.00000	0.00000	0.00522	0.00539	-0.63394
D30	2.59898	0.00000	0.00000	0.00758	0.00780	2.60677
D31	3.09001	0.00001	0.00000	0.01069	0.01073	3.10074
D32	0.04513	0.00001	0.00000	0.01305	0.01313	0.05826
D33	-0.17465	0.00003	0.00000	0.00494	0.00498	-0.16968
D34	2.51447	0.00002	0.00000	-0.00350	-0.00346	2.51101
D35	-2.62825	0.00001	0.00000	0.01059	0.01057	-2.61769
D36	0.06087	-0.00001	0.00000	0.00215	0.00213	0.06301
D37	-2.63460	-0.00002	0.00000	0.00507	0.00506	-2.62955
D38	0.52988	-0.00002	0.00000	0.00441	0.00440	0.53428
D39	-0.13446	0.00001	0.00000	-0.00080	-0.00079	-0.13526
D40	3.03001	0.00001	0.00000	-0.00146	-0.00145	3.02857
D41	0.03106	0.00001	0.00000	-0.00280	-0.00278	0.02828
D42	-3.10816	0.00000	0.00000	-0.00327	-0.00323	-3.11139
D43	2.75384	0.00000	0.00000	-0.01201	-0.01211	2.74174
D44	-0.38537	-0.00001	0.00000	-0.01248	-0.01256	-0.39793

This journal is © The Royal Society of Chemistry 2014

D45	3.11571	0.00000	0.00000	0.00090	0.00093	3.11664
D46	-0.02554	0.00000	0.00000	0.00229	0.00234	-0.02320
D47	0.01155	0.00001	0.00000	0.00546	0.00547	0.01702
D48	-3.12970	0.00001	0.00000	0.00685	0.00688	-3.12282
D49	-3.13285	0.00000	0.00000	-0.00041	-0.00043	-3.13328
D50	0.00688	0.00001	0.00000	0.00144	0.00146	0.00834
D51	0.00908	0.00000	0.00000	0.00099	0.00099	0.01007
D52	-3.13438	0.00001	0.00000	0.00284	0.00288	-3.13150
D53	0.02642	-0.00001	0.00000	-0.00180	-0.00184	0.02458
D54	-3.12899	-0.00001	0.00000	-0.00236	-0.00242	-3.13141
D55	-3.11704	0.00000	0.00000	0.00005	0.00005	-3.11699
D56	0.01073	0.00000	0.00000	-0.00051	-0.00053	0.01021
D57	0.03978	0.00000	0.00000	-0.00348	-0.00348	0.03630
D58	-3.05649	0.00002	0.00000	0.00577	0.00587	-3.05061
D59	3.08681	0.00000	0.00000	-0.00590	-0.00587	3.08094
D60	-0.00946	0.00001	0.00000	0.00335	0.00348	-0.00598
D61	3.07945	-0.00001	0.00000	-0.00433	-0.00443	3.07502
D62	-0.08635	0.00000	0.00000	-0.00288	-0.00294	-0.08928
D63	0.03779	-0.00001	0.00000	-0.00198	-0.00205	0.03574
D64	-3.12801	0.00000	0.00000	-0.00053	-0.00056	-3.12857
D65	0.03704	-0.00002	0.00000	0.01135	0.01122	0.04826
D66	-3.11756	0.00000	0.00000	0.00801	0.00795	-3.10961
D67	3.12903	-0.00003	0.00000	0.00121	0.00104	3.13007
D68	-0.02558	-0.00001	0.00000	-0.00212	-0.00223	-0.02780
D69	-3.10940	0.00000	0.00000	-0.00005	-0.00005	-3.10945
D70	0.03297	0.00000	0.00000	-0.00045	-0.00045	0.03252

```
   D71        0.01905   0.00002   0.00000  -0.00344  -0.00339
0.01566
   D72       -3.12176   0.00002   0.00000  -0.00384  -0.00379  -
3.12555
   D73        3.13903   0.00000   0.00000   0.00089   0.00089
3.13992
   D74       -0.00449   0.00001   0.00000   0.00187   0.00192  -
0.00256
   D75       -0.00178   0.00000   0.00000   0.00049   0.00049  -
0.00129
   D76        3.13789   0.00001   0.00000   0.00147   0.00152
3.13941
   D77       -0.03089   0.00000   0.00000  -0.00064  -0.00066  -
0.03155
   D78        3.13521  -0.00001   0.00000  -0.00210  -0.00217
3.13304
   D79        3.10878   0.00000   0.00000   0.00035   0.00037
3.10915
   D80       -0.00831   0.00000   0.00000  -0.00112  -0.00114  -
0.00945
   D81       -0.11858   0.00000   0.00000   0.00226   0.00224  -
0.11634
   D82        3.02092   0.00000   0.00000   0.00267   0.00264
3.02356
   D83        0.15669   0.00000   0.00000  -0.00086  -0.00085
0.15584
   D84       -3.00577   0.00000   0.00000  -0.00027  -0.00026  -
3.00603
         Item               Value     Threshold  Converged?
 Maximum Force            0.000104     0.000450     YES
 RMS     Force            0.000019     0.000300     YES
 Maximum Displacement     0.281912     0.001800     NO
 RMS     Displacement     0.028243     0.001200     NO
 Predicted change in Energy=-1.729114D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.553893    0.525544    1.165490
    2          6             0        0.610908    1.087607    0.501143
    3          6             0       -0.741962   -0.880578    1.059668
    4          6             0        0.225614   -1.601614    0.263903
    5          1             0        0.064490   -2.672414    0.148508
    6          6             0       -0.205369   -0.970051   -1.632184
    7          1             0        0.488387   -1.654354   -2.107025
    8          6             0       -0.099079    0.436634   -1.729760
    9          1             0        0.733330    0.989854   -2.142544
```

This journal is © The Royal Society of Chemistry 2014

10	6	0	-1.511163	1.283807	1.883877
11	1	0	-1.381986	2.352855	2.014539
12	6	0	-2.599127	0.658870	2.471562
13	1	0	-3.312778	1.249642	3.039154
14	6	0	-2.788537	-0.731519	2.343213
15	1	0	-3.650885	-1.205399	2.803471
16	6	0	-1.876264	-1.492299	1.631218
17	1	0	-2.017312	-2.563825	1.517808
18	6	0	1.598320	-1.141229	0.320582
19	6	0	1.805771	0.263210	0.419837
20	6	0	3.130834	0.759011	0.364865
21	1	0	3.301260	1.825810	0.428402
22	6	0	4.197758	-0.120320	0.250238
23	1	0	5.211502	0.271216	0.239404
24	6	0	3.985560	-1.509310	0.147572
25	1	0	4.832606	-2.184014	0.056867
26	6	0	2.693923	-2.012924	0.163631
27	1	0	2.516039	-3.082504	0.077165
28	6	0	-1.463839	0.986417	-1.792488
29	6	0	-1.664166	-1.283880	-1.726184
30	8	0	-2.367804	-0.088345	-1.694339
31	8	0	-2.214488	-2.350973	-1.795325
32	8	0	-1.856936	2.118311	-1.906827
33	6	0	0.628894	2.559930	0.262007
34	1	0	-0.370388	3.013942	0.149580
35	8	0	1.627246	3.249823	0.127843

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.453971	0.000000			
3	C	1.422584	2.452745	0.000000		
4	C	2.438297	2.727022	1.445454	0.000000	
5	H	3.412270	3.815847	2.165930	1.088985	0.000000
6	C	3.191434	3.074305	2.746271	2.044447	2.478251
7	H	4.067881	3.786279	3.484313	2.386028	2.510690
8	C	2.932104	2.429975	3.151072	2.869594	3.636045
9	H	3.579890	2.648325	3.991135	3.572739	4.371323
10	C	1.416831	2.540400	2.440400	3.737160	4.598465
11	H	2.178460	2.804076	3.431690	4.613776	5.552269
12	C	2.430346	3.790869	2.795068	4.238243	4.856839
13	H	3.412680	4.675796	3.881404	5.324650	5.928263
14	C	2.821503	4.273016	2.420367	3.763735	4.089446
15	H	3.907749	5.359241	3.407080	4.651197	4.796350
16	C	2.457083	3.757527	1.409792	2.509859	2.712495
17	H	3.436557	4.612386	2.160956	2.743874	2.494128
18	C	2.850267	2.444442	2.468016	1.448961	2.174113
19	C	2.488540	1.453940	2.865062	2.449241	3.423970
20	C	3.777925	2.544912	4.262576	3.744736	4.606946
21	H	4.134754	2.790740	4.906187	4.608025	5.548787
22	C	4.881906	3.793090	5.063003	4.239380	4.858748
23	H	5.844835	4.679794	6.119085	5.326085	5.930005

This journal is © The Royal Society of Chemistry 2014

24	C	5.077737	4.272852	4.855582	3.762877	4.089938
25	H	6.130670	5.359442	5.812087	4.648271	4.793940
26	C	4.242151	3.750489	3.726982	2.504352	2.710917
27	H	4.860755	4.604250	4.053191	2.733853	2.486635
28	C	3.128904	3.094440	3.484476	3.712263	4.414782
29	C	3.587269	3.970000	2.962108	2.762728	2.903575
30	O	3.441766	3.882748	3.294776	3.584761	3.998693
31	O	4.449534	5.008040	3.532900	3.279643	3.012566
32	O	3.697832	3.598739	4.363095	4.784028	5.555837
33	C	2.520713	1.491725	3.788483	4.181039	5.263920
34	H	2.694044	2.190274	4.016667	4.655281	5.702961
35	O	3.640848	2.418155	4.851974	5.051686	6.124992

		6	7	8	9	10
6	C	0.000000				
7	H	1.083994	0.000000			
8	C	1.414065	2.204467	0.000000		
9	H	2.232230	2.655766	1.081363	0.000000	
10	C	4.375804	5.343996	3.971153	4.619115	0.000000
11	H	5.071954	6.045106	4.397446	4.859390	1.084722
12	C	5.022369	5.987254	4.893949	5.701297	1.385491
13	H	6.033608	7.026038	5.807873	6.579397	2.140479
14	C	4.746940	5.603078	5.018653	5.957238	2.429859
15	H	5.621566	6.438020	5.988471	6.964448	3.408842
16	C	3.703299	4.426319	4.263255	5.216545	2.811388
17	H	3.968085	4.499453	4.819654	5.795933	3.898008
18	C	2.663812	2.718184	3.094304	3.369972	4.241884
19	C	3.126725	3.434761	2.877376	2.871226	3.766575
20	C	4.255363	4.349379	3.863123	3.476840	4.912326
21	H	4.935515	5.143169	4.260255	3.728652	5.056836
22	C	4.863444	4.655038	4.763758	4.354326	6.101813
23	H	5.863965	5.614389	5.666325	5.122904	6.994560
24	C	4.584999	4.163467	4.898504	4.697600	6.405484
25	H	5.450485	4.882131	5.863560	5.631598	7.457020
26	C	3.566291	3.185724	4.169667	4.263689	5.613416
27	H	3.845828	3.304795	4.742167	4.968828	6.208642
28	C	2.331783	3.299059	1.472674	2.224882	3.688678
29	C	1.495129	2.217155	2.325871	3.330346	4.432715
30	O	2.336106	3.283370	2.328942	3.313673	3.926865
31	O	2.443383	2.808554	3.500001	4.468928	5.219466
32	O	3.512988	4.446754	2.439150	2.835217	3.896845
33	C	4.092032	4.836553	3.000911	2.873658	2.973011
34	H	4.367392	5.255735	3.201257	3.250993	2.702318
35	O	4.925801	5.508411	3.787469	3.325838	4.098596

		11	12	13	14	15
11	H	0.000000				
12	C	2.135390	0.000000			
13	H	2.448443	1.086495	0.000000		
14	C	3.405845	1.409089	2.164293	0.000000	
15	H	4.293191	2.166069	2.489395	1.086298	0.000000
16	C	3.895697	2.419966	3.400603	1.384906	2.146105
17	H	4.982382	3.410853	4.305260	2.152540	2.483307
18	C	4.894930	5.048329	6.101294	4.848032	5.807151

This journal is © The Royal Society of Chemistry 2014

19	C	4.131765	4.875372	5.833817	5.079029	6.132995
20	C	5.062342	6.105788	6.993760	6.416736	7.469767
21	H	4.972564	6.352229	7.133968	6.876923	7.947421
22	C	6.353179	7.192986	8.127915	7.318636	8.324517
23	H	7.138516	8.132572	9.025479	8.332594	9.343272
24	C	6.871130	7.311636	8.320986	7.163392	8.090825
25	H	7.939572	8.315250	9.329057	8.088198	8.970570
26	C	6.252913	6.362500	7.415756	6.037379	6.919352
27	H	6.963558	6.774654	7.843213	6.229016	6.999087
28	C	4.045653	4.424736	5.180022	4.670134	5.541666
29	C	5.224794	4.719057	5.643146	4.257852	4.946816
30	O	4.548304	4.238699	5.008907	4.110051	4.808784
31	O	6.110165	5.235783	6.127223	4.481033	4.952222
32	O	3.956981	4.674517	5.228460	5.201179	6.037567
33	C	2.675422	4.349285	4.996616	5.181109	6.241253
34	H	2.222259	3.988138	4.485538	4.968697	5.967213
35	O	3.663284	5.483456	6.072915	6.344927	7.407203

		16	17	18	19	20
16	C	0.000000				
17	H	1.086704	0.000000			
18	C	3.730114	4.065700	0.000000		
19	C	4.255190	4.879922	1.423144	0.000000	
20	C	5.634100	6.234896	2.441613	1.415850	0.000000
21	H	6.266049	6.981612	3.422712	2.162932	1.082193
22	C	6.378336	6.797392	2.793615	2.428468	1.387331
23	H	7.435292	7.869405	3.880294	3.410517	2.140763
24	C	6.046691	6.246920	2.421638	2.822664	2.433732
25	H	6.925748	7.014269	3.408453	3.909268	3.413544
26	C	4.828195	4.932851	1.408841	2.456673	2.813363
27	H	4.923023	4.784950	2.161020	3.437399	3.901024
28	C	4.246869	4.885551	4.285879	4.013448	5.081034
29	C	3.370545	3.505204	3.854013	4.363411	5.615863
30	O	3.643080	4.070471	4.571500	4.691701	5.932399
31	O	3.548650	3.325813	4.525268	5.282366	6.550641
32	O	5.055161	5.803124	5.246404	4.719130	5.646781
33	C	4.956926	5.901890	3.826460	2.585512	3.084411
34	H	4.976859	5.974604	4.601141	3.517845	4.170086
35	O	6.084607	7.000951	4.395376	3.006158	2.919093

		21	22	23	24	25
21	H	0.000000				
22	C	2.150087	0.000000			
23	H	2.470123	1.086782	0.000000		
24	C	3.416161	1.408851	2.163710	0.000000	
25	H	4.308334	2.167777	2.490991	1.086710	0.000000
26	C	3.895490	2.418878	3.400183	1.386438	2.148170
27	H	4.983120	3.410670	4.305727	2.153924	2.484789
28	C	5.323824	6.119745	7.014291	6.299875	7.288138
29	C	6.242424	6.294622	7.318242	5.956608	6.796878
30	O	6.348882	6.847554	7.830359	6.765870	7.700938
31	O	7.267321	7.090631	8.133962	6.551629	7.288349
32	O	5.669730	6.806153	7.614518	7.177391	8.192439
33	C	2.776357	4.463257	5.122404	5.276269	6.341788

This journal is © The Royal Society of Chemistry 2014

34	H	3.869159	5.540910	6.219976	6.279657	7.355167
35	O	2.218214	4.240327	4.661699	5.311439	6.309196

		26	27	28	29	30
26	C	0.000000				
27	H	1.087713	0.000000			
28	C	5.487206	5.990922	0.000000		
29	C	4.805813	4.895021	2.280082	0.000000	
30	O	5.725132	5.996260	1.407800	1.387596	0.000000
31	O	5.295686	5.139966	3.420768	1.202632	2.270063
32	O	6.485693	7.078673	1.203654	3.412432	2.274966
33	C	5.018468	5.952524	3.328126	4.897540	4.452061
34	H	5.887239	6.745618	3.012992	4.864527	4.124791
35	O	5.369878	6.394599	4.285497	5.901294	5.515808

		31	32	33	34	35
31	O	0.000000				
32	O	4.484950	0.000000			
33	C	6.036092	3.328396	0.000000		
34	H	5.997139	2.690872	1.103327	0.000000	
35	O	7.058783	4.190432	1.220926	2.011629	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.512316	0.738542	1.047195
2	6	0	0.639769	1.143079	0.257840
3	6	0	-0.723610	-0.658516	1.212519
4	6	0	0.209016	-1.534832	0.540494
5	1	0	0.029162	-2.604897	0.632701
6	6	0	-0.270075	-1.261312	-1.428115
7	1	0	0.399125	-2.036020	-1.784543
8	6	0	-0.146661	0.099805	-1.791034
9	1	0	0.680705	0.549350	-2.322748
10	6	0	-1.436452	1.636718	1.635976
11	1	0	-1.288090	2.708553	1.559951
12	6	0	-2.514964	1.154553	2.359795
13	1	0	-3.202579	1.855176	2.825396
14	6	0	-2.728055	-0.231248	2.500083
15	1	0	-3.582772	-0.593387	3.064314
16	6	0	-1.848734	-1.129809	1.919268
17	1	0	-2.008474	-2.200612	2.013017
18	6	0	1.589257	-1.099169	0.472539
19	6	0	1.819701	0.294624	0.300559
20	6	0	3.149454	0.745091	0.117616
21	1	0	3.336978	1.801327	-0.025006
22	6	0	4.199723	-0.161032	0.141400

This journal is © The Royal Society of Chemistry 2014

```
   23          1             0        5.218176    0.201452    0.029798
   24          6             0        3.964653   -1.540197    0.307256
   25          1             0        4.798821   -2.236534    0.322034
   26          6             0        2.667018   -2.006288    0.452557
   27          1             0        2.471306   -3.069404    0.573391
   28          6             0       -1.504685    0.654932   -1.918990
   29          6             0       -1.735391   -1.558335   -1.422003
   30          8             0       -2.420557   -0.364353   -1.596287
   31          8             0       -2.302773   -2.608412   -1.274554
   32          8             0       -1.884820    1.752896   -2.233245
   33          6             0        0.671582    2.543879   -0.254009
   34          1             0       -0.324043    2.988424   -0.422654
   35          8             0        1.675189    3.176575   -0.542329
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3879084      0.2596126
0.2412264
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1905.5142592514 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A)

Harris functional with IExCor= 402 diagonalized for initial guess.
ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV=1
ScaDFX= 1.000000 1.000000 1.000000 1.000000
Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB+HF-LYP) = -1032.13789178 A.U. after 16 cycles
Convg = 0.8287D-08 -V/T = 2.0094
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000129049	-0.000276438	-0.000316069
2	6	-0.001141828	-0.000377433	0.000785643
3	6	0.000391971	0.000049259	-0.000285731
4	6	0.000270959	0.000221362	0.000223970
5	1	-0.000016656	0.000113021	-0.000165831
6	6	-0.000060617	0.000422690	-0.000023657
7	1	-0.000073586	0.000006470	-0.000006475
8	6	0.000083853	-0.000622290	-0.000040462
9	1	0.000036444	0.000224724	0.000693584
10	6	0.000176862	0.000038500	-0.000247214
11	1	0.000129475	0.000316189	-0.000398937
12	6	-0.000001792	0.000024739	0.000028108
13	1	0.000001324	-0.000007239	0.000008353
14	6	0.000057135	0.000006035	-0.000034897
15	1	-0.000007329	-0.000003663	-0.000013031

16	6	-0.000034978	0.000005641	0.000125743
17	1	-0.000000680	-0.000004251	0.000007913
18	6	-0.000429074	-0.000490661	0.000026113
19	6	-0.000544864	0.000214413	-0.000595200
20	6	0.000796060	0.000335846	-0.000078567
21	1	0.000064879	-0.000323846	-0.000003172
22	6	-0.000010948	0.000166922	0.000006182
23	1	0.000006769	-0.000033874	-0.000005286
24	6	-0.000398327	0.000070646	0.000054999
25	1	0.000002380	0.000031424	0.000008189
26	6	0.000338236	0.000109787	0.000027730
27	1	0.000034427	0.000014968	-0.000005244
28	6	0.000432293	-0.000465743	0.000193928
29	6	-0.000137143	0.000086602	-0.000093069
30	8	0.000032636	-0.000141813	0.000083124
31	8	0.000025296	0.000087939	-0.000001305
32	8	-0.000096321	0.000085288	-0.000080886
33	6	0.000625366	0.000403986	-0.000732080
34	1	-0.000290290	0.000321085	0.000791963
35	8	-0.000390979	-0.000610287	0.000061571

Cartesian Forces: Max 0.001141828 RMS 0.000300754

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Internal Forces: Max 0.001144594 RMS 0.000216696
Search for a saddle point.
Step number 7 out of a maximum of 202
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Swaping is turned off.
Update second derivatives using D2CorX and points 4 5 6 7
Eigenvalues --- -0.01889 0.00244 0.00606 0.00786
0.00860
Eigenvalues --- 0.01108 0.01262 0.01444 0.01483
0.01531
Eigenvalues --- 0.01630 0.01694 0.01774 0.01858
0.01922
Eigenvalues --- 0.01983 0.02113 0.02174 0.02190
0.02235
Eigenvalues --- 0.02361 0.02427 0.02449 0.02522
0.02681
Eigenvalues --- 0.02724 0.02746 0.02751 0.03197
0.03523
Eigenvalues --- 0.04124 0.05546 0.07028 0.07472
0.07620
Eigenvalues --- 0.08787 0.10194 0.11046 0.11179
0.11224
Eigenvalues --- 0.11861 0.12287 0.12499 0.12526
0.12660

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.12836   0.13903   0.14279   0.14663
0.16385
     Eigenvalues ---    0.17645   0.18502   0.19087   0.19174
0.19334
     Eigenvalues ---    0.19419   0.20106   0.20421   0.20901
0.21162
     Eigenvalues ---    0.23352   0.23904   0.24406   0.25103
0.26065
     Eigenvalues ---    0.27638   0.27927   0.29110   0.30148
0.30301
     Eigenvalues ---    0.31243   0.33089   0.33996   0.34044
0.35023
     Eigenvalues ---    0.35278   0.35919   0.36086   0.36134
0.36202
     Eigenvalues ---    0.36237   0.36329   0.36537   0.37434
0.37824
     Eigenvalues ---    0.38855   0.39859   0.40323   0.41121
0.42459
     Eigenvalues ---    0.44483   0.46400   0.47306   0.47637
0.50256
     Eigenvalues ---    0.50620   0.79396   0.89039
0.902561000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                          R1        R2        R3        R4        R5
          1             -0.04280   0.02341   0.15904   0.01774
0.37684
                          R6        R7        R8        R9        R10
          1              0.11148  -0.04441  -0.02054  -0.06077
0.19169
                          R11       R12       R13       R14       R15
          1              0.01900  -0.00684   0.43981   0.18106  -
0.05873
                          R16       R17       R18       R19       R20
          1              0.28817  -0.00745  -0.09423   0.18444  -
0.01294
                          R21       R22       R23       R24       R25
          1             -0.02857  -0.00730   0.16251  -0.00647  -
0.03439
                          R26       R27       R28       R29       R30
          1              0.07270  -0.00130  -0.01351   0.00007
0.01452
                          R31       R32       R33       R34       R35
          1             -0.00023  -0.01591  -0.00026   0.02080
0.01819
                          R36       R37       R38       R39       R40
          1              0.01707  -0.00114  -0.01221  -0.04525
0.00008
                          R41       R42       R43       R44       R45
          1              0.01347  -0.00013  -0.01512  -0.00013
0.00282
                          R46       R47       R48       R49       R50
          1              0.00093  -0.00183   0.00268  -0.00114
0.00513
                          A1        A2        A3        A4        A5
          1              0.02111  -0.00801  -0.01301   0.03230  -
0.00224
                          A6        A7        A8        A9        A10
          1              0.00537   0.01874  -0.00150  -0.01610
0.03351
                          A11       A12       A13       A14       A15
          1              0.05639   0.03018   0.06223   0.04273
0.02237
                          A16       A17       A18       A19       A20
          1              0.04741   0.00752   0.01721  -0.00382
0.00665
                          A21       A22       A23       A24       A25
```

This journal is © The Royal Society of Chemistry 2014

1	-0.00291	-0.00126	0.00481	-0.00355	-0.00141

	A26	A27	A28	A29	A30
1	-0.00119	0.00260	0.00407	-0.00652	0.00238

	A31	A32	A33	A34	A35
1	0.01922	-0.01724	-0.00100	0.02148	-0.00872

	A36	A37	A38	A39	A40
1	-0.01267	-0.00388	0.00667	-0.00281	-0.00098

	A41	A42	A43	A44	A45
1	0.00427	-0.00329	-0.00120	-0.00133	0.00253

	A46	A47	A48	A49	A50
1	0.00408	-0.00624	0.00207	-0.00257	0.00229

	A51	A52	A53	A54	A55
1	0.00027	-0.00669	0.00396	0.00282	-0.01364

	A56	A57	A58	D1	D2
1	-0.00084	0.00816	-0.00742	0.13362	-0.00624

	D3	D4	D5	D6	D7
1	0.12841	-0.01144	0.01890	0.00355	0.02381

	D8	D9	D10	D11	D12
1	0.00846	-0.00282	-0.00038	-0.00842	-0.00598

	D13	D14	D15	D16	D17
1	-0.13653	-0.13496	0.00998	0.01155	0.08510

	D18	D19	D20	D21	D22
1	0.08754	-0.06660	-0.06416	0.05117	-0.15920

	D23	D24	D25	D26	D27
1	0.06774	-0.14263	-0.00505	0.00100	-0.02309

	D28	D29	D30	D31	D32
1	-0.01704	0.15599	0.14472	-0.05652	-0.06779

	D33	D34	D35	D36	D37
1	0.01126	0.17650	-0.17070	-0.00545	-0.15007

	D38	D39	D40	D41	D42
1	-0.15465	0.02939	0.02482	-0.01954	-0.01682

	D43	D44	D45	D46	D47
1	0.14366	0.14638	-0.00126	-0.00032	0.00116

	D48	D49	D50	D51	D52

```
          1              0.00211   0.00005   0.00403   0.00100
0.00497
                           D53       D54       D55       D56       D57
          1             -0.00127  -0.00748   0.00271  -0.00350  -
0.01227
                           D58       D59       D60       D61       D62
          1             -0.01378  -0.00225  -0.00376   0.01431
0.00990
                           D63       D64       D65       D66       D67
          1              0.00160  -0.00281   0.00217   0.00025
0.00482
                           D68       D69       D70       D71       D72
          1              0.00290   0.00211   0.00041   0.00016  -
0.00154
                           D73       D74       D75       D76       D77
          1              0.00107  -0.00248  -0.00063  -0.00419
0.00149
                           D78       D79       D80       D81       D82
          1              0.00606  -0.00207   0.00250   0.04032
0.03793
                           D83       D84
          1             -0.04570  -0.04150
 RFO step:  Lambda0=3.430279379D-06 Lambda=-2.55277173D-04.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.02324445 RMS(Int)=  0.00125340
 Iteration  2 RMS(Cart)=  0.00160539 RMS(Int)=  0.00022416
 Iteration  3 RMS(Cart)=  0.00000454 RMS(Int)=  0.00022414
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00022414
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.74761  -0.00114   0.00000  -0.00050  -0.00051
2.74709
    R2        2.68829  -0.00025   0.00000   0.00000   0.00011
2.68840
    R3        5.54087  -0.00040   0.00000  -0.01681  -0.01679
5.52408
    R4        2.67742  -0.00052   0.00000  -0.00023  -0.00025
2.67718
    R5        4.59199   0.00021   0.00000  -0.03431  -0.03407
4.55791
    R6        5.00461  -0.00022   0.00000  -0.05218  -0.05194
4.95267
    R7        2.74755   0.00029   0.00000   0.00389   0.00309
2.75064
    R8        2.81895   0.00009   0.00000   0.00000  -0.00031
2.81864
    R9        2.73151   0.00004   0.00000  -0.00116  -0.00101
2.73050
   R10        5.18970   0.00014   0.00000   0.00513   0.00508
5.19478
```

This journal is © The Royal Society of Chemistry 2014

R11	2.66412	0.00007	0.00000	0.00054	0.00053
2.66465					
R12	2.05788	0.00003	0.00000	-0.00035	-0.00031
2.05758					
R13	3.86344	0.00005	0.00000	0.00787	0.00782
3.87127					
R14	4.50894	0.00021	0.00000	0.00486	0.00483
4.51377					
R15	2.73814	-0.00031	0.00000	-0.00155	-0.00141
2.73673					
R16	4.68321	-0.00021	0.00000	0.00476	0.00469
4.68790					
R17	2.04845	-0.00014	0.00000	-0.00027	-0.00027
2.04818					
R18	2.67220	-0.00039	0.00000	-0.00166	-0.00175
2.67045					
R19	5.03387	-0.00004	0.00000	0.00005	0.00011
5.03399					
R20	2.82538	0.00001	0.00000	-0.00079	-0.00079
2.82459					
R21	5.13662	-0.00006	0.00000	-0.00289	-0.00283
5.13379					
R22	2.04348	0.00003	0.00000	-0.00043	-0.00050
2.04298					
R23	5.43745	-0.00018	0.00000	-0.02690	-0.02708
5.41038					
R24	2.78295	-0.00029	0.00000	0.00100	0.00100
2.78395					
R25	5.42583	-0.00037	0.00000	-0.04514	-0.04517
5.38066					
R26	5.43043	0.00002	0.00000	-0.06101	-0.06130
5.36912					
R27	2.04983	0.00028	0.00000	-0.00017	-0.00017
2.04966					
R28	2.61820	-0.00004	0.00000	-0.00015	-0.00014
2.61806					
R29	2.05318	0.00000	0.00000	0.00001	0.00001
2.05319					
R30	2.66279	0.00015	0.00000	0.00000	0.00003
2.66282					
R31	2.05280	0.00000	0.00000	0.00001	0.00001
2.05282					
R32	2.61709	0.00015	0.00000	-0.00034	-0.00033
2.61677					
R33	2.05357	0.00000	0.00000	0.00003	0.00003
2.05361					
R34	2.68935	0.00017	0.00000	0.00049	0.00023
2.68959					
R35	2.66232	0.00001	0.00000	0.00004	0.00005
2.66238					
R36	2.67557	0.00076	0.00000	0.00193	0.00140
2.67697					

This journal is © The Royal Society of Chemistry 2014

R37	2.04505	-0.00032	0.00000	-0.00161	-0.00128
2.04377					
R38	2.62168	-0.00025	0.00000	-0.00025	-0.00025
2.62142					
R39	4.19182	-0.00002	0.00000	0.00340	0.00407
4.19589					
R40	2.05372	-0.00001	0.00000	-0.00004	-0.00004
2.05368					
R41	2.66234	-0.00008	0.00000	-0.00076	-0.00056
2.66178					
R42	2.05359	-0.00002	0.00000	-0.00001	-0.00001
2.05358					
R43	2.61999	-0.00025	0.00000	-0.00106	-0.00085
2.61913					
R44	2.05548	-0.00001	0.00000	-0.00006	-0.00006
2.05542					
R45	2.66036	-0.00008	0.00000	-0.00072	-0.00072
2.65963					
R46	2.27458	0.00012	0.00000	-0.00031	-0.00031
2.27426					
R47	2.62218	-0.00035	0.00000	-0.00028	-0.00027
2.62191					
R48	2.27265	-0.00009	0.00000	-0.00006	-0.00006
2.27259					
R49	2.08499	0.00031	0.00000	-0.00013	-0.00013
2.08485					
R50	2.30722	-0.00067	0.00000	-0.00088	-0.00072
2.30649					
A1	2.04207	0.00004	0.00000	-0.00095	-0.00110
2.04097					
A2	2.17251	-0.00073	0.00000	0.00072	0.00082
2.17333					
A3	2.06847	0.00069	0.00000	0.00011	0.00013
2.06860					
A4	2.05412	0.00024	0.00000	-0.00101	-0.00086
2.05326					
A5	2.05381	0.00003	0.00000	0.00447	0.00554
2.05935					
A6	2.14214	-0.00029	0.00000	-0.00468	-0.00597
2.13617					
A7	2.03255	0.00008	0.00000	0.00040	0.00038
2.03293					
A8	2.10029	-0.00041	0.00000	-0.00030	-0.00032
2.09997					
A9	2.14758	0.00033	0.00000	-0.00011	-0.00006
2.14752					
A10	2.03733	0.00005	0.00000	0.00124	0.00127
2.03860					
A11	2.04219	0.00002	0.00000	-0.00001	-0.00002
2.04218					
A12	2.04513	-0.00002	0.00000	0.00131	0.00133
2.04646					

This journal is © The Royal Society of Chemistry 2014

A13	2.15274	0.00001	0.00000	0.00188	0.00187
2.15461					
A14	2.05376	-0.00013	0.00000	0.00049	0.00051
2.05426					
A15	1.85231	0.00015	0.00000	0.00115	0.00114
1.85345					
A16	2.20573	0.00039	0.00000	0.00434	0.00420
2.20993					
A17	1.88037	-0.00018	0.00000	-0.00095	-0.00091
1.87946					
A18	2.10148	-0.00015	0.00000	-0.00030	-0.00024
2.10123					
A19	2.10373	-0.00021	0.00000	-0.00004	-0.00003
2.10371					
A20	2.09928	-0.00023	0.00000	0.00012	0.00009
2.09937					
A21	2.07940	0.00043	0.00000	0.00007	0.00008
2.07948					
A22	2.08531	0.00007	0.00000	0.00007	0.00006
2.08538					
A23	2.10830	-0.00013	0.00000	-0.00003	-0.00002
2.10828					
A24	2.08957	0.00006	0.00000	-0.00004	-0.00004
2.08953					
A25	2.09273	-0.00006	0.00000	0.00001	0.00000
2.09274					
A26	2.09477	0.00013	0.00000	-0.00004	-0.00002
2.09475					
A27	2.09568	-0.00007	0.00000	0.00003	0.00002
2.09570					
A28	2.09447	-0.00005	0.00000	0.00016	0.00015
2.09463					
A29	2.08285	0.00003	0.00000	-0.00005	-0.00004
2.08281					
A30	2.10577	0.00002	0.00000	-0.00011	-0.00010
2.10567					
A31	2.04248	-0.00012	0.00000	-0.00095	-0.00115
2.04133					
A32	2.13623	0.00021	0.00000	0.00023	0.00070
2.13693					
A33	2.10019	-0.00009	0.00000	0.00087	0.00060
2.10079					
A34	2.03048	-0.00013	0.00000	-0.00063	-0.00031
2.03017					
A35	2.18063	0.00025	0.00000	0.00289	0.00196
2.18259					
A36	2.07064	-0.00011	0.00000	-0.00185	-0.00127
2.06937					
A37	2.08323	0.00015	0.00000	0.00231	0.00183
2.08506					
A38	2.09554	-0.00004	0.00000	0.00070	0.00053
2.09606					

This journal is © The Royal Society of Chemistry 2014

A39	2.10430	-0.00012	0.00000	-0.00297	-0.00232	2.10198
A40	2.08270	0.00007	0.00000	0.00019	0.00026	2.08296
A41	2.11190	-0.00005	0.00000	-0.00003	-0.00017	2.11173
A42	2.08859	-0.00002	0.00000	-0.00016	-0.00009	2.08849
A43	2.09532	-0.00014	0.00000	-0.00028	-0.00033	2.09499
A44	2.09162	0.00023	0.00000	0.00029	0.00038	2.09200
A45	2.09625	-0.00010	0.00000	0.00000	-0.00005	2.09620
A46	2.09558	0.00006	0.00000	0.00002	-0.00008	2.09550
A47	2.08299	0.00000	0.00000	0.00012	0.00016	2.08316
A48	2.10438	-0.00006	0.00000	-0.00016	-0.00011	2.10427
A49	1.88292	0.00022	0.00000	0.00026	0.00024	1.88316
A50	2.28865	-0.00005	0.00000	-0.00018	-0.00017	2.28847
A51	2.11161	-0.00017	0.00000	-0.00008	-0.00007	2.11155
A52	1.88860	-0.00005	0.00000	-0.00031	-0.00032	1.88828
A53	2.26054	0.00005	0.00000	0.00035	0.00035	2.26089
A54	2.13384	-0.00001	0.00000	-0.00005	-0.00005	2.13379
A55	1.90769	-0.00014	0.00000	-0.00026	-0.00027	1.90742
A56	1.99496	0.00031	0.00000	0.00597	0.00646	2.00142
A57	2.19590	-0.00044	0.00000	-0.00337	-0.00436	2.19155
A58	2.09079	0.00017	0.00000	-0.00248	-0.00199	2.08880
D1	-0.56350	0.00011	0.00000	-0.00343	-0.00334	-0.56684
D2	2.84397	0.00024	0.00000	0.00209	0.00267	2.84664
D3	2.59608	0.00022	0.00000	0.00449	0.00444	2.60052
D4	-0.27964	0.00035	0.00000	0.01001	0.01045	-0.26919
D5	-0.03307	-0.00002	0.00000	0.00249	0.00248	-0.03059
D6	-3.09718	-0.00003	0.00000	0.00263	0.00256	-3.09463

This journal is © The Royal Society of Chemistry 2014

D7	3.09165	-0.00014	0.00000	-0.00493	-0.00481	3.08684
D8	0.02754	-0.00015	0.00000	-0.00479	-0.00473	0.02281
D9	-0.05565	0.00011	0.00000	0.00115	0.00123	-0.05442
D10	3.12850	0.00001	0.00000	-0.00294	-0.00288	3.12562
D11	3.10417	0.00023	0.00000	0.00919	0.00914	3.11332
D12	0.00514	0.00013	0.00000	0.00510	0.00503	0.01017
D13	0.55939	-0.00012	0.00000	0.00060	0.00057	0.55996
D14	-2.64074	0.00001	0.00000	0.00890	0.00885	-2.63189
D15	-2.86248	-0.00020	0.00000	-0.00369	-0.00380	-2.86628
D16	0.22057	-0.00007	0.00000	0.00461	0.00448	0.22504
D17	-0.49279	0.00078	0.00000	0.10970	0.10957	-0.38322
D18	2.70883	0.00002	0.00000	0.10750	0.10728	2.81611
D19	2.92904	0.00082	0.00000	0.11482	0.11493	3.04397
D20	-0.15253	0.00007	0.00000	0.11262	0.11264	-0.03988
D21	-3.10207	0.00006	0.00000	0.00696	0.00691	-3.09516
D22	0.62994	-0.00001	0.00000	0.00227	0.00213	0.63207
D23	-0.04026	0.00002	0.00000	0.00681	0.00682	-0.03344
D24	-2.59143	-0.00004	0.00000	0.00212	0.00204	-2.58939
D25	-0.04259	0.00008	0.00000	0.00145	0.00144	-0.04114
D26	3.11321	0.00004	0.00000	0.00088	0.00088	3.11410
D27	-3.10142	0.00009	0.00000	0.00158	0.00151	-3.09991
D28	0.05438	0.00005	0.00000	0.00101	0.00095	0.05533
D29	-0.63394	0.00012	0.00000	-0.00478	-0.00467	-0.63860
D30	2.60677	0.00012	0.00000	-0.00658	-0.00643	2.60034
D31	3.10074	0.00003	0.00000	-0.00947	-0.00944	3.09130
D32	0.05826	0.00004	0.00000	-0.01126	-0.01120	0.04706

This journal is © The Royal Society of Chemistry 2014

D33	-0.16968	0.00000	0.00000	-0.00368	-0.00366	-0.17334
D34	2.51101	0.00004	0.00000	0.00291	0.00294	2.51395
D35	-2.61769	0.00001	0.00000	-0.00845	-0.00847	-2.62615
D36	0.06301	0.00005	0.00000	-0.00185	-0.00186	0.06114
D37	-2.62955	-0.00011	0.00000	-0.00452	-0.00452	-2.63407
D38	0.53428	-0.00005	0.00000	-0.00397	-0.00397	0.53030
D39	-0.13526	-0.00006	0.00000	0.00056	0.00057	-0.13469
D40	3.02857	0.00000	0.00000	0.00111	0.00112	3.02968
D41	0.02828	-0.00004	0.00000	0.00254	0.00255	0.03083
D42	-3.11139	-0.00004	0.00000	0.00273	0.00276	-3.10863
D43	2.74174	0.00017	0.00000	0.01014	0.01008	2.75181
D44	-0.39793	0.00017	0.00000	0.01033	0.01028	-0.38765
D45	3.11664	-0.00001	0.00000	-0.00081	-0.00079	3.11585
D46	-0.02320	-0.00003	0.00000	-0.00210	-0.00207	-0.02527
D47	0.01702	-0.00009	0.00000	-0.00485	-0.00484	0.01218
D48	-3.12282	-0.00012	0.00000	-0.00614	-0.00612	-3.12895
D49	-3.13328	0.00002	0.00000	0.00041	0.00040	-3.13288
D50	0.00834	-0.00004	0.00000	-0.00135	-0.00133	0.00701
D51	0.01007	-0.00001	0.00000	-0.00089	-0.00089	0.00918
D52	-3.13150	-0.00007	0.00000	-0.00265	-0.00262	-3.13412
D53	0.02458	0.00003	0.00000	0.00166	0.00163	0.02621
D54	-3.13141	0.00007	0.00000	0.00224	0.00220	-3.12921
D55	-3.11699	-0.00003	0.00000	-0.00010	-0.00010	-3.11709
D56	0.01021	0.00001	0.00000	0.00048	0.00046	0.01067
D57	0.03630	0.00013	0.00000	0.00330	0.00330	0.03961
D58	-3.05061	0.00000	0.00000	-0.00461	-0.00452	-3.05514

This journal is © The Royal Society of Chemistry 2014

D59	3.08094	0.00014	0.00000	0.00502	0.00504	3.08598
D60	-0.00598	0.00001	0.00000	-0.00289	-0.00279	-0.00877
D61	3.07502	-0.00002	0.00000	0.00347	0.00338	3.07840
D62	-0.08928	-0.00001	0.00000	0.00225	0.00221	-0.08708
D63	0.03574	-0.00002	0.00000	0.00171	0.00166	0.03739
D64	-3.12857	0.00000	0.00000	0.00050	0.00048	-3.12809
D65	0.04826	-0.00008	0.00000	-0.00913	-0.00923	0.03903
D66	-3.10961	-0.00012	0.00000	-0.00662	-0.00667	-3.11628
D67	3.13007	0.00005	0.00000	-0.00061	-0.00075	3.12932
D68	-0.02780	0.00001	0.00000	0.00189	0.00181	-0.02599
D69	-3.10945	0.00001	0.00000	-0.00002	-0.00001	-3.10947
D70	0.03252	-0.00002	0.00000	0.00029	0.00030	0.03282
D71	0.01566	-0.00003	0.00000	0.00257	0.00261	0.01827
D72	-3.12555	-0.00006	0.00000	0.00288	0.00292	-3.12263
D73	3.13992	0.00001	0.00000	-0.00068	-0.00068	3.13924
D74	-0.00256	0.00001	0.00000	-0.00150	-0.00146	-0.00403
D75	-0.00129	-0.00001	0.00000	-0.00037	-0.00036	-0.00165
D76	3.13941	-0.00001	0.00000	-0.00119	-0.00115	3.13826
D77	-0.03155	0.00000	0.00000	0.00049	0.00048	-0.03107
D78	3.13304	-0.00002	0.00000	0.00172	0.00167	3.13470
D79	3.10915	0.00000	0.00000	-0.00033	-0.00031	3.10885
D80	-0.00945	-0.00001	0.00000	0.00089	0.00088	-0.00857
D81	-0.11634	0.00001	0.00000	-0.00216	-0.00217	-0.11851
D82	3.02356	0.00001	0.00000	-0.00232	-0.00235	3.02121
D83	0.15584	0.00000	0.00000	0.00094	0.00094	0.15679
D84	-3.00603	-0.00005	0.00000	0.00045	0.00045	-3.00558

This journal is © The Royal Society of Chemistry 2014

Item	Value	Threshold	Converged?
Maximum Force	0.001145	0.000450	NO
RMS Force	0.000217	0.000300	YES
Maximum Displacement	0.226458	0.001800	NO
RMS Displacement	0.023274	0.001200	NO

Predicted change in Energy=-1.338634D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.555665	0.523369	1.163851
2	6	0	0.605297	1.085830	0.493743
3	6	0	-0.741189	-0.883289	1.059918
4	6	0	0.225737	-1.603525	0.263613
5	1	0	0.063644	-2.673512	0.143668
6	6	0	-0.204154	-0.964936	-1.634835
7	1	0	0.490760	-1.647739	-2.109813
8	6	0	-0.096755	0.441422	-1.721957
9	1	0	0.737139	1.000922	-2.122402
10	6	0	-1.516078	1.281435	1.877982
11	1	0	-1.393171	2.352173	1.999819
12	6	0	-2.601653	0.655341	2.468667
13	1	0	-3.317411	1.246105	3.033618
14	6	0	-2.786866	-0.736096	2.345491
15	1	0	-3.647633	-1.210908	2.807756
16	6	0	-1.873685	-1.496287	1.634366
17	1	0	-2.012678	-2.568340	1.523256
18	6	0	1.597559	-1.142727	0.319247
19	6	0	1.802931	0.262550	0.412579
20	6	0	3.129022	0.758168	0.361885
21	1	0	3.301070	1.824327	0.419999
22	6	0	4.196632	-0.121100	0.255062
23	1	0	5.210369	0.270468	0.247480
24	6	0	3.985147	-1.510144	0.155764
25	1	0	4.832896	-2.184675	0.070546
26	6	0	2.694196	-2.014353	0.169010
27	1	0	2.517447	-3.084408	0.086602
28	6	0	-1.461979	0.991520	-1.784198
29	6	0	-1.662372	-1.278490	-1.732017
30	8	0	-2.365960	-0.083313	-1.692683
31	8	0	-2.212697	-2.345068	-1.808216
32	8	0	-1.854799	2.123794	-1.893880
33	6	0	0.629392	2.557480	0.252053
34	1	0	-0.362605	3.040303	0.250890
35	8	0	1.624577	3.220634	0.008007

Distance matrix (angstroms):

This journal is © The Royal Society of Chemistry 2014

		1	2	3	4	5
1	C	0.000000				
2	C	1.453699	0.000000			
3	C	1.422641	2.451736	0.000000		
4	C	2.438174	2.725739	1.444918	0.000000	
5	H	3.412384	3.814262	2.166142	1.088822	0.000000
6	C	3.189240	3.064588	2.748958	2.048587	2.480730
7	H	4.065168	3.776775	3.485582	2.388587	2.512532
8	C	2.923218	2.411943	3.147854	2.868502	3.634433
9	H	3.563545	2.620841	3.982821	3.568997	4.369225
10	C	1.416701	2.540593	2.440432	3.736723	4.598366
11	H	2.178252	2.804597	3.431720	4.613331	5.552037
12	C	2.430232	3.790801	2.795224	4.237791	4.857025
13	H	3.412568	4.675927	3.881588	5.324210	5.928469
14	C	2.821486	4.272605	2.420569	3.763300	4.089867
15	H	3.907737	5.358832	3.407299	4.650786	4.796890
16	C	2.457147	3.756821	1.410072	2.509589	2.713169
17	H	3.436673	4.611578	2.161195	2.743733	2.495083
18	C	2.850545	2.445711	2.466911	1.448215	2.174172
19	C	2.489058	1.455577	2.864357	2.447849	3.423140
20	C	3.778253	2.548320	4.261474	3.743837	4.606581
21	H	4.137658	2.796070	4.907193	4.607852	5.548679
22	C	4.881144	3.796226	5.060712	4.238592	4.858889
23	H	5.843872	4.683177	6.116556	5.325285	5.930140
24	C	5.076454	4.275125	4.852700	3.762115	4.090446
25	H	6.129063	5.361706	5.808863	4.647680	4.794797
26	C	4.241619	3.752344	3.724902	2.504200	2.711998
27	H	4.860097	4.605754	4.051047	2.734279	2.488622
28	C	3.119545	3.077587	3.481874	3.711627	4.413236
29	C	3.585742	3.960598	2.966423	2.766432	2.905755
30	O	3.435843	3.869848	3.294944	3.585392	3.998036
31	O	4.450490	5.001117	3.539537	3.284558	3.016530
32	O	3.687659	3.581926	4.359771	4.782920	5.553933
33	C	2.524548	1.491559	3.790781	4.180554	5.262612
34	H	2.684348	2.194488	4.023981	4.680966	5.730695
35	O	3.655772	2.415007	4.852375	5.029373	6.098841

		6	7	8	9	10
6	C	0.000000				
7	H	1.083850	0.000000			
8	C	1.413141	2.204586	0.000000		
9	H	2.233461	2.660125	1.081098	0.000000	
10	C	4.371180	5.339473	3.959756	4.599863	0.000000
11	H	5.062379	6.036354	4.379873	4.832888	1.084633
12	C	5.021158	5.985790	4.886882	5.687255	1.385416
13	H	6.031213	7.023631	5.799624	6.563843	2.140454
14	C	4.750344	5.605681	5.016710	5.949614	2.429794
15	H	5.626249	6.442019	5.988092	6.958799	3.408781
16	C	3.709089	4.430848	4.263461	5.212078	2.811222
17	H	3.976833	4.507094	4.822949	5.795856	3.897847
18	C	2.663872	2.716684	3.089781	3.361131	4.242753
19	C	3.118816	3.425414	2.863048	2.847320	3.768468
20	C	4.250416	4.342592	3.853357	3.457125	4.914194

This journal is © The Royal Society of Chemistry 2014

21	H	4.928380	5.133521	4.248013	3.703450	5.062150
22	C	4.863197	4.653681	4.760063	4.345038	6.102133
23	H	5.863991	5.613471	5.663344	5.114654	6.994689
24	C	4.588435	4.166834	4.898609	4.695215	6.404874
25	H	5.456002	4.888395	5.866081	5.633140	7.455885
26	C	3.571493	3.191014	4.170851	4.262924	5.613306
27	H	3.855207	3.315979	4.747254	4.973843	6.207975
28	C	2.330698	3.299228	1.473201	2.224992	3.674036
29	C	1.494711	2.216992	2.325802	3.332532	4.427947
30	O	2.335383	3.283638	2.329270	3.315033	3.915927
31	O	2.443168	2.808186	3.499883	4.471677	5.217744
32	O	3.511693	4.446655	2.439396	2.833939	3.879594
33	C	4.081980	4.825090	2.983573	2.841218	2.979089
34	H	4.429786	5.317790	3.273681	3.316779	2.659238
35	O	4.854089	5.428789	3.698618	3.202078	4.137755

		11	12	13	14	15
11	H	0.000000				
12	C	2.135296	0.000000			
13	H	2.448433	1.086500	0.000000		
14	C	3.405771	1.409103	2.164282	0.000000	
15	H	4.293123	2.166089	2.489372	1.086304	0.000000
16	C	3.895522	2.419813	3.400436	1.384734	2.145968
17	H	4.982203	3.410691	4.305057	2.152338	2.483071
18	C	4.897256	5.048410	6.101743	4.847082	5.805977
19	C	4.135326	4.876694	5.835677	5.079338	6.133238
20	C	5.066942	6.106532	6.995194	6.416015	7.468775
21	H	4.980999	6.356549	7.139303	6.879408	7.949750
22	C	6.356662	7.191633	8.127144	7.315556	8.320843
23	H	7.142193	8.130774	9.024271	8.328900	9.338827
24	C	6.873451	7.309225	8.319032	7.159204	8.085910
25	H	7.941599	8.311991	9.326176	8.082978	8.964370
26	C	6.254996	6.360951	7.414579	6.034322	6.915728
27	H	6.964894	6.772381	7.841162	6.225182	6.994491
28	C	4.021803	4.415737	5.169022	4.668438	5.542005
29	C	5.213519	4.718866	5.641277	4.264358	4.955338
30	O	4.529071	4.232965	5.001053	4.112194	4.813327
31	O	6.102198	5.238842	6.128643	4.491296	4.965134
32	O	3.927615	4.663257	5.214385	5.198075	6.036546
33	C	2.680969	4.355590	5.003405	5.186611	6.247024
34	H	2.143442	3.952204	4.437747	4.952331	5.949939
35	O	3.718649	5.522373	6.121792	6.370273	7.434606

		16	17	18	19	20
16	C	0.000000				
17	H	1.086721	0.000000			
18	C	3.728818	4.063967	0.000000		
19	C	4.254853	4.879182	1.423268	0.000000	
20	C	5.632837	6.233099	2.441434	1.416589	0.000000
21	H	6.267317	6.982022	3.422793	2.164169	1.081514
22	C	6.375137	6.793588	2.793389	2.429363	1.387197
23	H	7.431601	7.865039	3.880034	3.411444	2.140782
24	C	6.042546	6.242092	2.421218	2.823201	2.433244
25	H	6.920813	7.008527	3.408066	3.909806	3.412974

26	C	4.825059	4.929051	1.408870	2.457227	2.813032
27	H	4.919324	4.780412	2.161121	3.437866	3.900667
28	C	4.247972	4.890310	4.282554	4.002108	5.073205
29	C	3.380033	3.518981	3.853994	4.356882	5.611582
30	O	3.648025	4.079514	4.569432	4.683097	5.926564
31	O	3.561843	3.344930	4.526563	5.277960	6.547776
32	O	5.055083	5.806709	5.242793	4.707757	5.638429
33	C	4.960767	5.905126	3.825362	2.582570	3.081839
34	H	4.977752	5.983188	4.620028	3.525848	4.172758
35	O	6.093622	7.002701	4.374531	2.990944	2.907287

		21	22	23	24	25
21	H	0.000000				
22	C	2.148004	0.000000			
23	H	2.467724	1.086759	0.000000		
24	C	3.414158	1.408555	2.163368	0.000000	
25	H	4.305892	2.167307	2.490284	1.086708	0.000000
26	C	3.894452	2.418497	3.399661	1.385986	2.147730
27	H	4.982058	3.410167	4.304986	2.153424	2.484167
28	C	5.314009	6.116893	7.011980	6.300235	7.290661
29	C	6.236538	6.294121	7.317940	5.959182	6.801391
30	O	6.341746	6.845637	7.828803	6.766769	7.703780
31	O	7.262949	7.091026	8.134422	6.554966	7.293549
32	O	5.659214	6.802744	7.611625	7.177152	8.194336
33	C	2.775533	4.460942	5.120136	5.274080	6.339592
34	H	3.863898	5.548074	6.223346	6.294327	7.370627
35	O	2.220369	4.224179	4.649594	5.289081	6.286062

		26	27	28	29	30
26	C	0.000000				
27	H	1.087681	0.000000			
28	C	5.488541	5.995742	0.000000		
29	C	4.809894	4.903020	2.279435	0.000000	
30	O	5.727128	6.001675	1.407417	1.387455	0.000000
31	O	5.300603	5.148905	3.420084	1.202603	2.269884
32	O	6.486381	7.082671	1.203487	3.411563	2.274442
33	C	5.017167	5.951725	3.312458	4.889108	4.441612
34	H	5.907646	6.770065	3.089938	4.926792	4.189019
35	O	5.345567	6.368434	4.208060	5.837279	5.452779

		31	32	33	34	35
31	O	0.000000				
32	O	4.483989	0.000000			
33	C	6.029689	3.311241	0.000000		
34	H	6.055161	2.768876	1.103257	0.000000	
35	O	7.000026	4.114158	1.220543	2.010076	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

This journal is © The Royal Society of Chemistry 2014

Number	Number	Type	X	Y	Z
1	6	0	-0.519877	0.695639	1.076904
2	6	0	0.629255	1.133603	0.301711
3	6	0	-0.724032	-0.707723	1.190047
4	6	0	0.213254	-1.553785	0.487577
5	1	0	0.035917	-2.627076	0.533741
6	6	0	-0.259445	-1.200522	-1.474175
7	1	0	0.414868	-1.957281	-1.858034
8	6	0	-0.138441	0.175093	-1.774191
9	1	0	0.690859	0.655518	-2.274419
10	6	0	-1.452397	1.566682	1.692315
11	1	0	-1.314170	2.641594	1.648866
12	6	0	-2.528996	1.052761	2.396727
13	1	0	-3.222807	1.732335	2.883847
14	6	0	-2.733176	-0.338443	2.488556
15	1	0	-3.586742	-0.725473	3.037819
16	6	0	-1.847813	-1.210419	1.877590
17	1	0	-2.001850	-2.284779	1.932233
18	6	0	1.591207	-1.110742	0.439785
19	6	0	1.814905	0.289366	0.315887
20	6	0	3.144727	0.751589	0.158893
21	1	0	3.330337	1.811676	0.051950
22	6	0	4.199094	-0.149869	0.159301
23	1	0	5.216652	0.220697	0.068189
24	6	0	3.969311	-1.534730	0.275014
25	1	0	4.806803	-2.227210	0.271393
26	6	0	2.673526	-2.011593	0.395427
27	1	0	2.482531	-3.079102	0.479059
28	6	0	-1.498506	0.730317	-1.884961
29	6	0	-1.723187	-1.502917	-1.487456
30	8	0	-2.411884	-0.304801	-1.610929
31	8	0	-2.287400	-2.560385	-1.389072
32	8	0	-1.881221	1.839191	-2.153864
33	6	0	0.663640	2.551861	-0.158843
34	1	0	-0.322499	3.044064	-0.208269
35	8	0	1.659478	3.155750	-0.524013

```
 Rotational constants (GHZ):      0.3889838      0.2596445
0.2419789
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1906.8007839079 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
```

This journal is © The Royal Society of Chemistry 2014

```
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
```

This journal is © The Royal Society of Chemistry 2014

```
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1032.13801609     A.U. after   16 cycles
            Convg  =    0.6456D-08             -V/T =  2.0093
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000015627    0.000018324   -0.000061253
    2          6           0.000002561   -0.000019234   -0.000093002
    3          6          -0.000011678   -0.000005082   -0.000006181
    4          6           0.000010873   -0.000004748    0.000049596
    5          1          -0.000000427   -0.000008093   -0.000001351
    6          6          -0.000002398    0.000025503   -0.000053781
    7          1           0.000008723   -0.000003082   -0.000001462
    8          6           0.000020379   -0.000022090    0.000067822
    9          1           0.000008122    0.000018735    0.000100217
   10          6           0.000001691    0.000003612    0.000008493
   11          1           0.000010268    0.000008559    0.000006169
   12          6           0.000001414    0.000000667   -0.000001845
   13          1          -0.000000313   -0.000003472    0.000001419
   14          6           0.000000994   -0.000006587    0.000002296
   15          1           0.000000503   -0.000003128   -0.000000962
   16          6           0.000004744   -0.000003881   -0.000002634
   17          1           0.000002220   -0.000002069   -0.000002970
   18          6           0.000007538    0.000006559   -0.000006998
   19          6          -0.000044481    0.000020093   -0.000021108
   20          6          -0.000001989   -0.000003886    0.000020259
   21          1          -0.000008050    0.000017814   -0.000025423
   22          6          -0.000001082    0.000002585    0.000001404
   23          1          -0.000000277    0.000004212    0.000002061
   24          6           0.000007395    0.000002812   -0.000000764
   25          1           0.000001538    0.000003296   -0.000001408
   26          6          -0.000000919   -0.000001576    0.000005311
   27          1           0.000002025    0.000001173   -0.000001734
   28          6          -0.000004811    0.000012015    0.000003500
   29          6          -0.000003135   -0.000002613    0.000006928
   30          8           0.000000156    0.000000589    0.000007877
   31          8           0.000003233   -0.000001375   -0.000001400
   32          8          -0.000003516   -0.000006368   -0.000008641
   33          6           0.000036164   -0.000048022   -0.000049711
   34          1          -0.000011804   -0.000017898    0.000045525
   35          8          -0.000020033    0.000016658    0.000013753
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000100217 RMS     0.000021994


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000050028 RMS     0.000012367
```

This journal is © The Royal Society of Chemistry 2014

```
 Search for a saddle point.
 Step number   8 out of a maximum of 202
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Update second derivatives using D2CorX and points  4  5  6  7  8

     Eigenvalues ---   -0.01888   0.00252   0.00592   0.00814
0.00861
     Eigenvalues ---    0.01055   0.01262   0.01444   0.01487
0.01534
     Eigenvalues ---    0.01636   0.01693   0.01774   0.01868
0.01926
     Eigenvalues ---    0.01988   0.02110   0.02174   0.02190
0.02237
     Eigenvalues ---    0.02361   0.02427   0.02449   0.02523
0.02678
     Eigenvalues ---    0.02723   0.02746   0.02751   0.03186
0.03518
     Eigenvalues ---    0.04096   0.05546   0.07030   0.07468
0.07609
     Eigenvalues ---    0.08786   0.10185   0.11046   0.11179
0.11224
     Eigenvalues ---    0.11859   0.12285   0.12499   0.12527
0.12659
     Eigenvalues ---    0.12835   0.13904   0.14283   0.14663
0.16389
     Eigenvalues ---    0.17650   0.18505   0.19087   0.19173
0.19334
     Eigenvalues ---    0.19417   0.20109   0.20423   0.20903
0.21163
     Eigenvalues ---    0.23351   0.23905   0.24404   0.25102
0.26063
     Eigenvalues ---    0.27641   0.27928   0.29105   0.30148
0.30312
     Eigenvalues ---    0.31240   0.33085   0.33996   0.34024
0.35016
     Eigenvalues ---    0.35277   0.35919   0.36086   0.36133
0.36202
     Eigenvalues ---    0.36237   0.36329   0.36535   0.37426
0.37818
     Eigenvalues ---    0.38853   0.39858   0.40323   0.41123
0.42459
     Eigenvalues ---    0.44484   0.46391   0.47305   0.47637
0.50257
     Eigenvalues ---    0.50619   0.79385   0.89039
0.902561000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
         1             -0.04270   0.02330   0.15646   0.01779
0.37213
                           R6        R7        R8        R9        R10
         1              0.10876  -0.04342  -0.02018  -0.06104
0.19280
                           R11       R12       R13       R14       R15
         1              0.01906  -0.00699   0.44294   0.18322  -
0.05902
                           R16       R17       R18       R19       R20
         1              0.29169  -0.00746  -0.09393   0.18537  -
0.01327
                           R21       R22       R23       R24       R25
         1             -0.02819  -0.00702   0.15966  -0.00607  -
0.03466
                           R26       R27       R28       R29       R30
         1              0.07462  -0.00133  -0.01351   0.00007
0.01444
                           R31       R32       R33       R34       R35
```

This journal is © The Royal Society of Chemistry 2014

1	-0.00023	-0.01598	-0.00025	0.02101	0.01825

	R36	R37	R38	R39	R40
1	0.01758	-0.00147	-0.01220	-0.04858	0.00008

	R41	R42	R43	R44	R45
1	0.01323	-0.00013	-0.01538	-0.00013	0.00248

	R46	R47	R48	R49	R50
1	0.00091	-0.00161	0.00268	-0.00125	0.00497

	A1	A2	A3	A4	A5
1	0.02120	-0.00790	-0.01319	0.03224	-0.00320

	A6	A7	A8	A9	A10
1	0.00649	0.01904	-0.00140	-0.01649	0.03308

	A11	A12	A13	A14	A15
1	0.05686	0.02977	0.06209	0.04256	0.02259

	A16	A17	A18	A19	A20
1	0.04652	0.00717	0.01621	-0.00372	0.00678

	A21	A22	A23	A24	A25
1	-0.00313	-0.00130	0.00483	-0.00353	-0.00136

	A26	A27	A28	A29	A30
1	-0.00129	0.00265	0.00414	-0.00659	0.00237

	A31	A32	A33	A34	A35
1	0.01959	-0.01794	-0.00070	0.02119	-0.00780

	A36	A37	A38	A39	A40
1	-0.01334	-0.00347	0.00691	-0.00346	-0.00107

	A41	A42	A43	A44	A45
1	0.00442	-0.00335	-0.00112	-0.00149	0.00261

	A46	A47	A48	A49	A50
1	0.00421	-0.00633	0.00202	-0.00239	0.00204

	A51	A52	A53	A54	A55
1	0.00035	-0.00665	0.00411	0.00263	-0.01363

	A56	A57	A58	D1	D2
1	-0.00125	0.00909	-0.00794	0.13293	-0.00521

	D3	D4	D5	D6	D7
1	0.12827	-0.00987	0.01961	0.00429	0.02402

	D8	D9	D10	D11	D12

```
          1              0.00870  -0.00342  -0.00092  -0.00861  -
0.00612
                           D13       D14       D15       D16       D17
          1             -0.13606  -0.13520   0.00722   0.00808
0.08303
                           D18       D19       D20       D21       D22
          1              0.08555  -0.06621  -0.06369   0.05184  -
0.15973
                           D23       D24       D25       D26       D27
          1              0.06841  -0.14317  -0.00516   0.00091  -
0.02320
                           D28       D29       D30       D31       D32
          1             -0.01713   0.15635   0.14511  -0.05737  -
0.06861
                           D33       D34       D35       D36       D37
          1              0.01447   0.17756  -0.16915  -0.00606  -
0.15095
                           D38       D39       D40       D41       D42
          1             -0.15572   0.02985   0.02508  -0.01898  -
0.01648
                           D43       D44       D45       D46       D47
          1              0.14161   0.14411  -0.00126  -0.00040
0.00121
                           D48       D49       D50       D51       D52
          1              0.00208   0.00017   0.00418   0.00104
0.00504
                           D53       D54       D55       D56       D57
          1             -0.00134  -0.00756   0.00267  -0.00355  -
0.01262
                           D58       D59       D60       D61       D62
          1             -0.01351  -0.00268  -0.00357   0.01419
0.00983
                           D63       D64       D65       D66       D67
          1              0.00154  -0.00283   0.00282   0.00093
0.00461
                           D68       D69       D70       D71       D72
          1              0.00272   0.00206   0.00048   0.00015  -
0.00143
                           D73       D74       D75       D76       D77
          1              0.00104  -0.00245  -0.00055  -0.00403
0.00145
                           D78       D79       D80       D81       D82
          1              0.00598  -0.00204   0.00249   0.04008
0.03789
                           D83       D84
          1             -0.04579  -0.04141
 RFO step:  Lambda0=1.509328079D-11 Lambda=-1.72348394D-06.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.00193170 RMS(Int)=  0.00000584
 Iteration  2 RMS(Cart)=  0.00000746 RMS(Int)=  0.00000108
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000108
```

This journal is © The Royal Society of Chemistry 2014

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.74709	-0.00003	0.00000	0.00035	0.00035	2.74745
R2	2.68840	0.00000	0.00000	0.00010	0.00010	2.68850
R3	5.52408	-0.00003	0.00000	-0.00290	-0.00290	5.52118
R4	2.67718	0.00000	0.00000	-0.00001	-0.00001	2.67717
R5	4.55791	-0.00002	0.00000	-0.00625	-0.00625	4.55166
R6	4.95267	-0.00004	0.00000	-0.00726	-0.00726	4.94541
R7	2.75064	-0.00004	0.00000	-0.00005	-0.00005	2.75059
R8	2.81864	-0.00004	0.00000	-0.00027	-0.00027	2.81837
R9	2.73050	0.00000	0.00000	-0.00017	-0.00017	2.73033
R10	5.19478	0.00001	0.00000	0.00184	0.00184	5.19662
R11	2.66465	0.00000	0.00000	0.00006	0.00006	2.66471
R12	2.05758	0.00000	0.00000	0.00001	0.00001	2.05759
R13	3.87127	0.00001	0.00000	0.00378	0.00378	3.87505
R14	4.51377	0.00002	0.00000	0.00243	0.00243	4.51620
R15	2.73673	0.00001	0.00000	-0.00012	-0.00012	2.73661
R16	4.68790	0.00001	0.00000	0.00382	0.00382	4.69172
R17	2.04818	0.00000	0.00000	-0.00004	-0.00004	2.04814
R18	2.67045	-0.00001	0.00000	-0.00019	-0.00019	2.67026
R19	5.03399	0.00000	0.00000	0.00127	0.00127	5.03526
R20	2.82459	0.00000	0.00000	-0.00035	-0.00035	2.82425
R21	5.13379	-0.00001	0.00000	-0.00022	-0.00022	5.13357
R22	2.04298	0.00000	0.00000	-0.00006	-0.00007	2.04291
R23	5.41038	-0.00002	0.00000	-0.00381	-0.00381	5.40657
R24	2.78395	0.00001	0.00000	0.00046	0.00046	2.78441

This journal is © The Royal Society of Chemistry 2014

R25	5.38066	-0.00003	0.00000	-0.00475	-0.00475
5.37590					
R26	5.36912	-0.00002	0.00000	-0.00884	-0.00884
5.36028					
R27	2.04966	0.00001	0.00000	-0.00003	-0.00003
2.04963					
R28	2.61806	0.00000	0.00000	0.00003	0.00003
2.61809					
R29	2.05319	0.00000	0.00000	0.00000	0.00000
2.05319					
R30	2.66282	0.00001	0.00000	-0.00001	-0.00001
2.66281					
R31	2.05282	0.00000	0.00000	0.00000	0.00000
2.05281					
R32	2.61677	0.00001	0.00000	-0.00005	-0.00005
2.61672					
R33	2.05361	0.00000	0.00000	0.00000	0.00000
2.05361					
R34	2.68959	-0.00001	0.00000	-0.00010	-0.00010
2.68948					
R35	2.66238	0.00000	0.00000	0.00003	0.00003
2.66241					
R36	2.67697	-0.00001	0.00000	-0.00022	-0.00023
2.67674					
R37	2.04377	0.00002	0.00000	0.00009	0.00009
2.04385					
R38	2.62142	0.00000	0.00000	0.00007	0.00007
2.62149					
R39	4.19589	0.00001	0.00000	-0.00079	-0.00079
4.19510					
R40	2.05368	0.00000	0.00000	0.00000	0.00000
2.05368					
R41	2.66178	0.00001	0.00000	0.00002	0.00002
2.66181					
R42	2.05358	0.00000	0.00000	0.00000	0.00000
2.05358					
R43	2.61913	0.00001	0.00000	0.00006	0.00006
2.61919					
R44	2.05542	0.00000	0.00000	0.00000	0.00000
2.05542					
R45	2.65963	0.00000	0.00000	-0.00030	-0.00030
2.65933					
R46	2.27426	0.00000	0.00000	-0.00007	-0.00007
2.27420					
R47	2.62191	0.00000	0.00000	0.00030	0.00030
2.62221					
R48	2.27259	0.00000	0.00000	0.00000	0.00000
2.27259					
R49	2.08485	0.00000	0.00000	-0.00010	-0.00010
2.08475					
R50	2.30649	-0.00001	0.00000	0.00005	0.00005
2.30654					

This journal is © The Royal Society of Chemistry 2014

A1	2.04097	0.00000	0.00000	-0.00025	-0.00025
2.04072					
A2	2.17333	-0.00001	0.00000	0.00040	0.00040
2.17374					
A3	2.06860	0.00002	0.00000	-0.00016	-0.00016
2.06845					
A4	2.05326	0.00002	0.00000	-0.00027	-0.00027
2.05299					
A5	2.05935	-0.00005	0.00000	0.00020	0.00020
2.05955					
A6	2.13617	0.00002	0.00000	-0.00030	-0.00030
2.13586					
A7	2.03293	-0.00001	0.00000	0.00009	0.00009
2.03301					
A8	2.09997	-0.00001	0.00000	0.00010	0.00010
2.10007					
A9	2.14752	0.00001	0.00000	-0.00014	-0.00014
2.14737					
A10	2.03860	0.00000	0.00000	0.00026	0.00026
2.03886					
A11	2.04218	0.00000	0.00000	0.00022	0.00022
2.04240					
A12	2.04646	0.00000	0.00000	0.00027	0.00027
2.04673					
A13	2.15461	0.00000	0.00000	0.00049	0.00049
2.15510					
A14	2.05426	0.00000	0.00000	0.00049	0.00049
2.05475					
A15	1.85345	0.00000	0.00000	0.00030	0.00030
1.85375					
A16	2.20993	0.00001	0.00000	-0.00003	-0.00003
2.20990					
A17	1.87946	0.00000	0.00000	-0.00020	-0.00020
1.87926					
A18	2.10123	-0.00001	0.00000	-0.00010	-0.00010
2.10113					
A19	2.10371	0.00000	0.00000	0.00015	0.00015
2.10386					
A20	2.09937	-0.00001	0.00000	0.00005	0.00005
2.09942					
A21	2.07948	0.00001	0.00000	-0.00020	-0.00020
2.07928					
A22	2.08538	0.00000	0.00000	-0.00007	-0.00007
2.08531					
A23	2.10828	0.00000	0.00000	0.00008	0.00008
2.10836					
A24	2.08953	0.00000	0.00000	-0.00001	-0.00001
2.08951					
A25	2.09274	0.00000	0.00000	0.00002	0.00002
2.09276					
A26	2.09475	0.00000	0.00000	-0.00007	-0.00007
2.09468					

This journal is © The Royal Society of Chemistry 2014

A27	2.09570	0.00000	0.00000	0.00005	0.00005
2.09575					
A28	2.09463	0.00000	0.00000	-0.00001	-0.00001
2.09462					
A29	2.08281	0.00000	0.00000	-0.00003	-0.00003
2.08278					
A30	2.10567	0.00000	0.00000	0.00004	0.00004
2.10571					
A31	2.04133	-0.00001	0.00000	-0.00010	-0.00010
2.04123					
A32	2.13693	0.00001	0.00000	0.00013	0.00014
2.13707					
A33	2.10079	0.00000	0.00000	-0.00001	-0.00001
2.10078					
A34	2.03017	0.00000	0.00000	0.00007	0.00007
2.03024					
A35	2.18259	-0.00002	0.00000	-0.00018	-0.00019
2.18240					
A36	2.06937	0.00001	0.00000	0.00012	0.00012
2.06949					
A37	2.08506	-0.00001	0.00000	-0.00012	-0.00012
2.08494					
A38	2.09606	-0.00001	0.00000	-0.00004	-0.00005
2.09602					
A39	2.10198	0.00001	0.00000	0.00017	0.00017
2.10215					
A40	2.08296	0.00000	0.00000	-0.00001	-0.00001
2.08294					
A41	2.11173	0.00000	0.00000	-0.00001	-0.00001
2.11173					
A42	2.08849	0.00000	0.00000	0.00002	0.00002
2.08851					
A43	2.09499	0.00000	0.00000	0.00000	0.00000
2.09499					
A44	2.09200	0.00000	0.00000	-0.00001	0.00000
2.09200					
A45	2.09620	0.00000	0.00000	0.00000	0.00000
2.09620					
A46	2.09550	0.00000	0.00000	-0.00006	-0.00006
2.09545					
A47	2.08316	0.00000	0.00000	0.00002	0.00002
2.08318					
A48	2.10427	0.00000	0.00000	0.00004	0.00004
2.10431					
A49	1.88316	0.00000	0.00000	-0.00001	-0.00001
1.88315					
A50	2.28847	0.00000	0.00000	-0.00016	-0.00016
2.28832					
A51	2.11155	0.00000	0.00000	0.00016	0.00016
2.11171					
A52	1.88828	0.00000	0.00000	-0.00007	-0.00007
1.88821					

This journal is © The Royal Society of Chemistry 2014

A53	2.26089	0.00000	0.00000	0.00020	0.00020	2.26109
A54	2.13379	0.00000	0.00000	-0.00013	-0.00013	2.13366
A55	1.90742	0.00000	0.00000	0.00002	0.00002	1.90744
A56	2.00142	-0.00005	0.00000	0.00006	0.00007	2.00149
A57	2.19155	0.00005	0.00000	-0.00003	-0.00004	2.19151
A58	2.08880	0.00001	0.00000	-0.00005	-0.00005	2.08875
D1	-0.56684	0.00000	0.00000	-0.00129	-0.00129	-0.56812
D2	2.84664	0.00001	0.00000	0.00018	0.00018	2.84682
D3	2.60052	-0.00001	0.00000	-0.00118	-0.00118	2.59934
D4	-0.26919	0.00000	0.00000	0.00029	0.00029	-0.26890
D5	-0.03059	0.00001	0.00000	0.00140	0.00140	-0.02919
D6	-3.09463	0.00000	0.00000	0.00075	0.00075	-3.09387
D7	3.08684	0.00001	0.00000	0.00131	0.00131	3.08816
D8	0.02281	0.00001	0.00000	0.00066	0.00066	0.02347
D9	-0.05442	0.00000	0.00000	-0.00067	-0.00067	-0.05509
D10	3.12562	0.00000	0.00000	-0.00059	-0.00059	3.12503
D11	3.11332	-0.00001	0.00000	-0.00056	-0.00056	3.11276
D12	0.01017	-0.00001	0.00000	-0.00048	-0.00048	0.00969
D13	0.55996	0.00000	0.00000	0.00063	0.00063	0.56060
D14	-2.63189	0.00000	0.00000	0.00075	0.00075	-2.63115
D15	-2.86628	-0.00003	0.00000	-0.00082	-0.00082	-2.86710
D16	0.22504	-0.00003	0.00000	-0.00071	-0.00071	0.22434
D17	-0.38322	0.00003	0.00000	0.00663	0.00663	-0.37659
D18	2.81611	-0.00002	0.00000	0.00700	0.00700	2.82311
D19	3.04397	0.00005	0.00000	0.00816	0.00816	3.05213
D20	-0.03988	0.00000	0.00000	0.00854	0.00854	-0.03135

This journal is © The Royal Society of Chemistry 2014

D21	-3.09516	0.00000	0.00000	0.00055	0.00055	-3.09461
D22	0.63207	-0.00001	0.00000	-0.00079	-0.00079	0.63128
D23	-0.03344	0.00001	0.00000	0.00124	0.00124	-0.03220
D24	-2.58939	0.00000	0.00000	-0.00011	-0.00011	-2.58950
D25	-0.04114	0.00000	0.00000	-0.00035	-0.00035	-0.04150
D26	3.11410	0.00000	0.00000	-0.00016	-0.00016	3.11394
D27	-3.09991	-0.00001	0.00000	-0.00106	-0.00106	-3.10097
D28	0.05533	-0.00001	0.00000	-0.00086	-0.00086	0.05447
D29	-0.63860	0.00000	0.00000	0.00010	0.00010	-0.63851
D30	2.60034	0.00000	0.00000	-0.00021	-0.00021	2.60014
D31	3.09130	-0.00001	0.00000	-0.00125	-0.00125	3.09005
D32	0.04706	0.00000	0.00000	-0.00155	-0.00155	0.04551
D33	-0.17334	0.00000	0.00000	0.00171	0.00171	-0.17163
D34	2.51395	0.00000	0.00000	0.00092	0.00092	2.51488
D35	-2.62615	-0.00001	0.00000	-0.00017	-0.00017	-2.62633
D36	0.06114	-0.00001	0.00000	-0.00096	-0.00096	0.06018
D37	-2.63407	0.00000	0.00000	-0.00103	-0.00103	-2.63510
D38	0.53030	-0.00001	0.00000	-0.00110	-0.00110	0.52920
D39	-0.13469	0.00001	0.00000	0.00073	0.00073	-0.13396
D40	3.02968	0.00000	0.00000	0.00066	0.00066	3.03034
D41	0.03083	0.00001	0.00000	0.00090	0.00090	0.03173
D42	-3.10863	0.00001	0.00000	0.00092	0.00092	-3.10771
D43	2.75181	0.00001	0.00000	0.00020	0.00020	2.75201
D44	-0.38765	0.00001	0.00000	0.00022	0.00022	-0.38743
D45	3.11585	0.00000	0.00000	-0.00004	-0.00004	3.11581
D46	-0.02527	0.00000	0.00000	-0.00001	-0.00001	-0.02529

This journal is © The Royal Society of Chemistry 2014

D47	0.01218	0.00000	0.00000	0.00003	0.00003	0.01220
D48	-3.12895	0.00000	0.00000	0.00006	0.00006	-3.12889
D49	-3.13288	0.00000	0.00000	0.00014	0.00014	-3.13273
D50	0.00701	0.00000	0.00000	0.00034	0.00034	0.00734
D51	0.00918	0.00000	0.00000	0.00017	0.00017	0.00936
D52	-3.13412	0.00000	0.00000	0.00036	0.00036	-3.13375
D53	0.02621	0.00000	0.00000	-0.00015	-0.00015	0.02606
D54	-3.12921	0.00000	0.00000	-0.00035	-0.00035	-3.12956
D55	-3.11709	0.00000	0.00000	0.00004	0.00004	-3.11705
D56	0.01067	0.00000	0.00000	-0.00016	-0.00016	0.01051
D57	0.03961	0.00001	0.00000	-0.00011	-0.00011	0.03950
D58	-3.05514	0.00000	0.00000	-0.00020	-0.00020	-3.05534
D59	3.08598	0.00001	0.00000	0.00020	0.00020	3.08617
D60	-0.00877	0.00000	0.00000	0.00010	0.00010	-0.00867
D61	3.07840	0.00000	0.00000	0.00030	0.00030	3.07870
D62	-0.08708	0.00000	0.00000	0.00028	0.00028	-0.08680
D63	0.03739	0.00000	0.00000	-0.00001	-0.00001	0.03738
D64	-3.12809	0.00000	0.00000	-0.00003	-0.00003	-3.12812
D65	0.03903	-0.00002	0.00000	-0.00082	-0.00082	0.03821
D66	-3.11628	-0.00001	0.00000	-0.00028	-0.00028	-3.11656
D67	3.12932	-0.00001	0.00000	-0.00071	-0.00071	3.12862
D68	-0.02599	0.00000	0.00000	-0.00017	-0.00017	-0.02616
D69	-3.10947	0.00000	0.00000	0.00004	0.00004	-3.10943
D70	0.03282	0.00000	0.00000	0.00014	0.00014	0.03296
D71	0.01827	0.00001	0.00000	0.00058	0.00058	0.01885
D72	-3.12263	0.00001	0.00000	0.00068	0.00068	-3.12195

```
   D73        3.13924   0.00000   0.00000  -0.00009  -0.00009
3.13915
   D74       -0.00403   0.00000   0.00000  -0.00005  -0.00004  -
0.00407
   D75       -0.00165   0.00000   0.00000   0.00002   0.00002  -
0.00164
   D76        3.13826   0.00000   0.00000   0.00006   0.00006
3.13832
   D77       -0.03107   0.00000   0.00000  -0.00002  -0.00002  -
0.03109
   D78        3.13470   0.00000   0.00000   0.00000   0.00000
3.13471
   D79        3.10885   0.00000   0.00000   0.00002   0.00002
3.10887
   D80       -0.00857   0.00000   0.00000   0.00005   0.00005  -
0.00852
   D81       -0.11851   0.00000   0.00000  -0.00042  -0.00042  -
0.11893
   D82        3.02121   0.00000   0.00000  -0.00044  -0.00044
3.02077
   D83        0.15679   0.00000   0.00000  -0.00018  -0.00018
0.15660
   D84       -3.00558   0.00000   0.00000  -0.00011  -0.00011  -
3.00569
         Item               Value     Threshold  Converged?
 Maximum Force            0.000050     0.000450     YES
 RMS     Force            0.000012     0.000300     YES
 Maximum Displacement     0.018166     0.001800     NO
 RMS     Displacement     0.001932     0.001200     NO
 Predicted change in Energy=-8.620610D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.555929    0.523103    1.163462
    2          6             0        0.604717    1.085271    0.492155
    3          6             0       -0.741527   -0.883617    1.059790
    4          6             0        0.225666   -1.604210    0.264292
    5          1             0        0.063406   -2.674137    0.143991
    6          6             0       -0.203744   -0.963918   -1.635850
    7          1             0        0.491831   -1.646353   -2.110339
    8          6             0       -0.096350    0.442475   -1.720724
    9          1             0        0.737584    1.002567   -2.120160
   10          6             0       -1.515935    1.281038    1.878267
   11          1             0       -1.392970    2.351703    2.000534
   12          6             0       -2.601338    0.654915    2.469277
   13          1             0       -3.316694    1.245670    3.034749
```

This journal is © The Royal Society of Chemistry 2014

14	6	0	-2.786907	-0.736444	2.345831
15	1	0	-3.647618	-1.211193	2.808263
16	6	0	-1.873980	-1.496610	1.634400
17	1	0	-2.012976	-2.568664	1.523291
18	6	0	1.597377	-1.143236	0.319552
19	6	0	1.802445	0.262103	0.411776
20	6	0	3.128276	0.758061	0.360963
21	1	0	3.299812	1.824428	0.417601
22	6	0	4.196187	-0.121035	0.255275
23	1	0	5.209814	0.270819	0.247620
24	6	0	3.985099	-1.510231	0.157095
25	1	0	4.833049	-2.184609	0.072674
26	6	0	2.694247	-2.014776	0.170369
27	1	0	2.517761	-3.084939	0.088822
28	6	0	-1.461883	0.992419	-1.783380
29	6	0	-1.661697	-1.277706	-1.733433
30	8	0	-2.365580	-0.082550	-1.693131
31	8	0	-2.211963	-2.344238	-1.810678
32	8	0	-1.854691	2.124712	-1.892531
33	6	0	0.629261	2.556731	0.250238
34	1	0	-0.361896	3.041112	0.256417
35	8	0	1.623611	3.218270	-0.001606

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.453885	0.000000			
3	C	1.422693	2.451754	0.000000		
4	C	2.438208	2.725602	1.444830	0.000000	
5	H	3.412512	3.814103	2.166233	1.088827	0.000000
6	C	3.189265	3.062873	2.749933	2.050587	2.482751
7	H	4.064740	3.774585	3.486066	2.389872	2.514337
8	C	2.921685	2.408634	3.147385	2.869304	3.635376
9	H	3.561634	2.616999	3.982153	3.569728	4.370246
10	C	1.416695	2.541022	2.440357	3.736676	4.598417
11	H	2.178326	2.805318	3.431715	4.613433	5.552193
12	C	2.430273	3.791174	2.795108	4.237635	4.856995
13	H	3.412572	4.676321	3.881471	5.324055	5.928444
14	C	2.821652	4.272923	2.420566	3.763166	4.089870
15	H	3.907902	5.359147	3.407320	4.650654	4.796900
16	C	2.457291	3.756962	1.410102	2.509439	2.713181
17	H	3.436785	4.611594	2.161204	2.743495	2.494985
18	C	2.850543	2.445692	2.466947	1.448151	2.174292
19	C	2.488992	1.455548	2.864331	2.447674	3.423080
20	C	3.777906	2.548064	4.261319	3.743636	4.606570
21	H	4.137209	2.795613	4.906968	4.607542	5.548539
22	C	4.880812	3.796043	5.060612	4.238505	4.859074
23	H	5.843476	4.682954	6.116437	5.325199	5.930348
24	C	5.076234	4.275030	4.852679	3.762135	4.090786
25	H	6.128834	5.361611	5.808862	4.647748	4.795229
26	C	4.241546	3.752329	3.724934	2.504253	2.712339
27	H	4.860081	4.605764	4.051118	2.734419	2.489108

This journal is © The Royal Society of Chemistry 2014

28	C	3.118476	3.075308	3.481672	3.712582	4.414171
29	C	3.585755	3.958982	2.967173	2.767608	2.907013
30	O	3.435371	3.868067	3.295122	3.586294	3.998914
31	O	4.450798	4.999826	3.540506	3.285601	3.017759
32	O	3.686601	3.579924	4.359515	4.783788	5.554770
33	C	2.524737	1.491416	3.790835	4.180492	5.262458
34	H	2.683421	2.194362	4.024055	4.682340	5.732154
35	O	3.656734	2.414877	4.852413	5.028048	6.097204

		6	7	8	9	10
6	C	0.000000				
7	H	1.083828	0.000000			
8	C	1.413039	2.204759	0.000000		
9	H	2.233320	2.660314	1.081064	0.000000	
10	C	4.371577	5.339449	3.958680	4.598186	0.000000
11	H	5.062696	6.036241	4.378828	4.831102	1.084617
12	C	5.022065	5.986352	4.886328	5.686141	1.385432
13	H	6.032183	7.024286	5.799161	6.562725	2.140429
14	C	4.751658	5.606737	5.016554	5.949057	2.429860
15	H	5.627748	6.443372	5.988143	6.958455	3.408839
16	C	3.710523	4.431992	4.263435	5.211801	2.811226
17	H	3.978530	4.508656	4.823282	5.796034	3.897854
18	C	2.664543	2.716566	3.089647	3.360939	4.242571
19	C	3.117803	3.423591	2.861034	2.844805	3.768352
20	C	4.249098	4.340436	3.851134	3.454151	4.913697
21	H	4.926098	5.130455	4.244543	3.698743	5.061644
22	C	4.862735	4.652416	4.758991	4.343628	6.101496
23	H	5.863331	5.612030	5.662087	5.112991	6.993944
24	C	4.589065	4.166858	4.898724	4.695359	6.404295
25	H	5.456961	4.888910	5.866586	5.633777	7.455232
26	C	3.572826	3.191865	4.171541	4.263732	5.612927
27	H	3.857436	3.318166	4.748756	4.975574	6.207622
28	C	2.330651	3.299549	1.473446	2.225125	3.673402
29	C	1.494528	2.217125	2.325832	3.332530	4.428634
30	O	2.335299	3.283952	2.329338	3.315036	3.916140
31	O	2.443111	2.808441	3.499954	4.471769	5.218755
32	O	3.511573	4.446857	2.439508	2.833887	3.878848
33	C	4.079975	4.822564	2.980148	2.836537	2.979889
34	H	4.432375	5.320029	3.276051	3.318529	2.657078
35	O	4.847749	5.421461	3.690348	3.191026	4.140476

		11	12	13	14	15
11	H	0.000000				
12	C	2.135173	0.000000			
13	H	2.448188	1.086501	0.000000		
14	C	3.405722	1.409097	2.164269	0.000000	
15	H	4.293029	2.166096	2.489375	1.086303	0.000000
16	C	3.895502	2.419737	3.400368	1.384710	2.145975
17	H	4.982187	3.410649	4.305036	2.152341	2.483131
18	C	4.897191	5.048155	6.101415	4.846982	5.805883
19	C	4.135367	4.876569	5.835493	5.079352	6.133265
20	C	5.066513	6.106071	6.994608	6.415812	7.468600
21	H	4.980552	6.356156	7.138808	6.879265	7.949658
22	C	6.356024	7.190984	8.126300	7.315241	8.320545

This journal is © The Royal Society of Chemistry 2014

23	H	7.141397	8.130030	9.023290	8.328543	9.338488
24	C	6.872876	7.308570	8.318177	7.158867	8.085573
25	H	7.940912	8.311240	9.325182	8.082584	8.963967
26	C	6.254677	6.360460	7.413947	6.034055	6.915453
27	H	6.964591	6.771872	7.840506	6.224871	6.994153
28	C	4.021245	4.415582	5.169026	4.668516	5.542250
29	C	5.214147	4.720246	5.642872	4.266082	4.957350
30	O	4.529318	4.233802	5.002163	4.113187	4.814562
31	O	6.103110	5.240663	6.130746	4.493565	4.967848
32	O	3.926915	4.662956	5.214236	5.197976	6.036582
33	C	2.682348	4.356353	5.004293	5.187169	6.247595
34	H	2.140173	3.950416	4.435490	4.951390	5.948949
35	O	3.722803	5.525057	6.125130	6.372040	7.436489

		16	17	18	19	20
16	C	0.000000				
17	H	1.086723	0.000000			
18	C	3.728809	4.063924	0.000000		
19	C	4.254877	4.879154	1.423214	0.000000	
20	C	5.632739	6.233023	2.441372	1.416469	0.000000
21	H	6.267218	6.981943	3.422708	2.164025	1.081560
22	C	6.375039	6.793560	2.793356	2.429256	1.387232
23	H	7.431494	7.865030	3.880004	3.411332	2.140806
24	C	6.042468	6.242089	2.421217	2.823120	2.433280
25	H	6.920735	7.008555	3.408076	3.909725	3.413014
26	C	4.824996	4.929010	1.408887	2.457187	2.813064
27	H	4.919247	4.780357	2.161146	3.437829	3.900697
28	C	4.248095	4.890715	4.282806	4.000989	5.071755
29	C	3.381610	3.520827	3.854140	4.355826	5.610231
30	O	3.648794	4.080498	4.569571	4.682077	5.925233
31	O	3.563884	3.347433	4.526738	5.277100	6.546635
32	O	5.055055	5.806951	5.243050	4.706781	5.637015
33	C	4.961017	5.905232	3.825155	2.582203	3.080998
34	H	4.977565	5.983362	4.620769	3.525819	4.171877
35	O	6.094239	7.002762	4.373393	2.990282	2.906562

		21	22	23	24	25
21	H	0.000000				
22	C	2.148177	0.000000			
23	H	2.467935	1.086760	0.000000		
24	C	3.414298	1.408567	2.163390	0.000000	
25	H	4.306062	2.167320	2.490318	1.086707	0.000000
26	C	3.894525	2.418530	3.399704	1.386016	2.147757
27	H	4.982127	3.410212	4.305053	2.153474	2.484233
28	C	5.311337	6.116343	7.011221	6.300660	7.291407
29	C	6.234321	6.293461	7.317115	5.959402	6.801928
30	O	6.339434	6.845038	7.828025	6.767033	7.704348
31	O	7.261038	7.090499	8.133750	6.555248	7.294154
32	O	5.656482	6.802174	7.610808	7.177529	8.195008
33	C	2.774188	4.460203	5.119264	5.273566	6.339059
34	H	3.861917	5.547548	6.222423	6.294517	7.370846
35	O	2.219950	4.223161	4.648702	5.287771	6.284673

		26	27	28	29	30
26	C	0.000000				

```
   27  H    1.087679   0.000000
   28  C    5.489425   5.997296   0.000000
   29  C    4.810612   4.904546   2.279449   0.000000
   30  O    5.727825   6.003058   1.407257   1.387614   0.000000
   31  O    5.301320   5.150439   3.420037   1.202602   2.269945
   32  O    6.487200   7.084106   1.203453   3.411599   2.274373
   33  C    5.016894   5.951548   3.309918   4.887366   4.439770
   34  H    5.908419   6.771189   3.093200   4.929622   4.191986
   35  O    5.344212   6.366955   4.201119   5.831490   5.447046
                 31         32         33         34         35
   31  O    0.000000
   32  O    4.483956   0.000000
   33  C    6.028219   3.308794   0.000000
   34  H    6.057856   2.772400   1.103202   0.000000
   35  O    6.994703   4.107317   1.220570   2.010025   0.000000
Stoichiometry    C19H12O4
Framework group  C1[X(C19H12O4)]
Deg. of freedom    99
Full point group                 C1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0       -0.520652    0.691320    1.079465
   2          6             0        0.628099    1.132140    0.304976
   3          6             0       -0.724264   -0.712556    1.187761
   4          6             0        0.213842   -1.555889    0.483289
   5          1             0        0.036805   -2.629411    0.525181
   6          6             0       -0.258134   -1.194326   -1.479213
   7          1             0        0.417283   -1.948964   -1.865241
   8          6             0       -0.137634    0.182782   -1.772014
   9          1             0        0.691631    0.666118   -2.269411
  10          6             0       -1.453278    1.559675    1.698489
  11          1             0       -1.315461    2.634790    1.659388
  12          6             0       -2.529618    1.042743    2.401125
  13          1             0       -3.223428    1.720300    2.891051
  14          6             0       -2.733550   -0.348834    2.487613
  15          1             0       -3.586999   -0.738145    3.035442
  16          6             0       -1.847920   -1.218212    1.873396
  17          1             0       -2.001485   -2.292834    1.924124
  18          6             0        1.591486   -1.111933    0.437009
  19          6             0        1.814245    0.288618    0.317120
  20          6             0        3.143633    0.752328    0.161930
  21          1             0        3.328237    1.812877    0.057379
  22          6             0        4.198739   -0.148316    0.160402
  23          1             0        5.216041    0.223311    0.070741
  24          6             0        3.969984   -1.533682    0.272179
  25          1             0        4.808012   -2.225501    0.267002
  26          6             0        2.674485   -2.011892    0.390658
```

This journal is © The Royal Society of Chemistry 2014

```
   27          1             0        2.484238   -3.079767    0.471253
   28          6             0       -1.498247    0.737578   -1.881458
   29          6             0       -1.721484   -1.497628   -1.494278
   30          8             0       -2.410966   -0.299260   -1.612605
   31          8             0       -2.285206   -2.555808   -1.400881
   32          8             0       -1.881379    1.847340   -2.145914
   33          6             0        0.662383    2.551841   -0.150652
   34          1             0       -0.322919    3.046376   -0.191504
   35          8             0        1.656971    3.154769   -0.520873
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3890066      0.2596502
0.2420687
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1906.9044323688 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1032.13801795     A.U. after   14 cycles
            Convg  =    0.5534D-08             -V/T =  2.0093
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.000002458   -0.000004282   -0.000019303
    2          6          -0.000062490   -0.000027241   -0.000013055
    3          6           0.000023809   -0.000000925   -0.000009212
    4          6           0.000023970    0.000010222    0.000041024
    5          1          -0.000001408    0.000003785   -0.000011221
    6          6          -0.000004349    0.000029933   -0.000042820
    7          1          -0.000001132   -0.000000894    0.000001517
    8          6           0.000001576   -0.000025040    0.000039308
    9          1           0.000007413    0.000017683    0.000036319
   10          6           0.000007614    0.000000733   -0.000006873
   11          1           0.000012528    0.000010322   -0.000007259
   12          6          -0.000001235   -0.000003107    0.000000379
   13          1          -0.000000844   -0.000003828    0.000001036
   14          6           0.000003105   -0.000002154   -0.000000468
   15          1           0.000000252   -0.000003633   -0.000001345
   16          6          -0.000000054   -0.000000983    0.000001980
   17          1           0.000001329   -0.000002083   -0.000001398
   18          6          -0.000023941   -0.000024025    0.000004688
   19          6          -0.000028811    0.000002758   -0.000012353
   20          6           0.000055653    0.000004943    0.000003988
   21          1           0.000019340   -0.000028562   -0.000010225
   22          6          -0.000002598    0.000009449    0.000001442
   23          1           0.000000400    0.000000474    0.000000462
   24          6          -0.000021071    0.000006115    0.000000972
```

```
   25          1           0.000001119    0.000004041   -0.000000417
   26          6           0.000022701    0.000006117   -0.000001242
   27          1           0.000004339    0.000001764   -0.000001579
   28          6           0.000008710   -0.000008610   -0.000001391
   29          6          -0.000003377    0.000004097    0.000000174
   30          8           0.000001780   -0.000008332    0.000005007
   31          8           0.000002515    0.000003057   -0.000000913
   32          8          -0.000003950   -0.000001333    0.000000108
   33          6           0.000022678    0.000007392   -0.000050533
   34          1          -0.000021320    0.000016304    0.000018266
   35          8          -0.000046706    0.000005841    0.000034933
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000062490 RMS     0.000017231


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000055730 RMS     0.000010947
 Search for a saddle point.
 Step number   9 out of a maximum of 202
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Update second derivatives using D2CorX and points  4  5  6  7  8
                                                      9
     Eigenvalues ---   -0.01888   0.00224   0.00492   0.00781
0.00857
     Eigenvalues ---    0.01039   0.01264   0.01443   0.01486
0.01536
     Eigenvalues ---    0.01640   0.01692   0.01775   0.01876
0.01929
     Eigenvalues ---    0.01992   0.02115   0.02175   0.02189
0.02238
     Eigenvalues ---    0.02362   0.02428   0.02449   0.02523
0.02674
     Eigenvalues ---    0.02721   0.02746   0.02750   0.03146
0.03512
     Eigenvalues ---    0.04045   0.05546   0.07030   0.07452
0.07520
     Eigenvalues ---    0.08785   0.10179   0.11044   0.11179
0.11223
     Eigenvalues ---    0.11857   0.12281   0.12499   0.12527
0.12658
     Eigenvalues ---    0.12834   0.13903   0.14272   0.14664
0.16391
     Eigenvalues ---    0.17650   0.18503   0.19087   0.19171
0.19333
     Eigenvalues ---    0.19415   0.20109   0.20412   0.20901
0.21163
     Eigenvalues ---    0.23351   0.23905   0.24400   0.25102
0.26062
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.27640   0.27927   0.29101   0.30147
0.30311
     Eigenvalues ---    0.31234   0.33077   0.33992   0.34008
0.35007
     Eigenvalues ---    0.35275   0.35918   0.36086   0.36133
0.36202
     Eigenvalues ---    0.36237   0.36329   0.36535   0.37410
0.37812
     Eigenvalues ---    0.38852   0.39856   0.40319   0.41121
0.42458
     Eigenvalues ---    0.44481   0.46325   0.47304   0.47637
0.50256
     Eigenvalues ---    0.50618   0.79376   0.89039
0.902561000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
```

This journal is © The Royal Society of Chemistry 2014

	R1	R2	R3	R4	R5
1	-0.04244	0.02325	0.15116	0.01775	0.36257

	R6	R7	R8	R9	R10
1	0.09996	-0.04309	-0.02016	-0.06152	0.19539

	R11	R12	R13	R14	R15
1	0.01915	-0.00703	0.44882	0.18728	-0.05942

	R16	R17	R18	R19	R20
1	0.29751	-0.00755	-0.09410	0.18715	-0.01383

	R21	R22	R23	R24	R25
1	-0.02836	-0.00697	0.15374	-0.00542	-0.03983

	R26	R27	R28	R29	R30
1	0.06859	-0.00133	-0.01348	0.00007	0.01443

	R31	R32	R33	R34	R35
1	-0.00024	-0.01604	-0.00025	0.02104	0.01838

	R36	R37	R38	R39	R40
1	0.01767	-0.00150	-0.01219	-0.05011	0.00008

	R41	R42	R43	R44	R45
1	0.01319	-0.00013	-0.01548	-0.00013	0.00198

	R46	R47	R48	R49	R50
1	0.00085	-0.00118	0.00268	-0.00129	0.00487

	A1	A2	A3	A4	A5
1	0.02106	-0.00769	-0.01326	0.03199	-0.00388

	A6	A7	A8	A9	A10
1	0.00666	0.01912	-0.00135	-0.01658	0.03333

	A11	A12	A13	A14	A15
1	0.05731	0.03005	0.06279	0.04306	0.02300

	A16	A17	A18	A19	A20
1	0.04623	0.00683	0.01581	-0.00366	0.00680

	A21	A22	A23	A24	A25
1	-0.00322	-0.00134	0.00488	-0.00354	-0.00135

	A26	A27	A28	A29	A30
1	-0.00134	0.00269	0.00412	-0.00661	0.00241

	A31	A32	A33	A34	A35
1	0.01960	-0.01803	-0.00062	0.02107	-0.00754

	A36	A37	A38	A39	A40

This journal is © The Royal Society of Chemistry 2014

1	-0.01351	-0.00347	0.00698	-0.00352	-0.00108

	A41	A42	A43	A44	A45
1	0.00446	-0.00337	-0.00110	-0.00152	0.00262

	A46	A47	A48	A49	A50
1	0.00422	-0.00635	0.00204	-0.00233	0.00175

	A51	A52	A53	A54	A55
1	0.00058	-0.00671	0.00441	0.00240	-0.01364

	A56	A57	A58	D1	D2
1	-0.00139	0.00929	-0.00798	0.13149	-0.00301

	D3	D4	D5	D6	D7
1	0.12670	-0.00779	0.02142	0.00531	0.02595

	D8	D9	D10	D11	D12
1	0.00985	-0.00438	-0.00167	-0.00971	-0.00700

	D13	D14	D15	D16	D17
1	-0.13548	-0.13538	0.00379	0.00389	0.08291

	D18	D19	D20	D21	D22
1	0.08475	-0.06244	-0.06060	0.05296	-0.16096

	D23	D24	D25	D26	D27
1	0.07034	-0.14358	-0.00574	0.00064	-0.02462

	D28	D29	D30	D31	D32
1	-0.01824	0.15674	0.14545	-0.05932	-0.07061

	D33	D34	D35	D36	D37
1	0.01871	0.17899	-0.16790	-0.00761	-0.15265

	D38	D39	D40	D41	D42
1	-0.15761	0.03099	0.02604	-0.01751	-0.01527

	D43	D44	D45	D46	D47
1	0.14053	0.14276	-0.00125	-0.00035	0.00144

	D48	D49	D50	D51	D52
1	0.00233	0.00041	0.00472	0.00131	0.00562

	D53	D54	D55	D56	D57
1	-0.00161	-0.00815	0.00271	-0.00383	-0.01280

	D58	D59	D60	D61	D62
1	-0.01299	-0.00282	-0.00300	0.01406	0.00981

	D63	D64	D65	D66	D67

```
          1              0.00136  -0.00290   0.00244   0.00114
0.00345
                         D68       D69       D70       D71       D72
          1              0.00215   0.00206   0.00068   0.00076  -
0.00063
                         D73       D74       D75       D76       D77
          1              0.00099  -0.00224  -0.00041  -0.00364
0.00124
                         D78       D79       D80       D81       D82
          1              0.00567  -0.00199   0.00243   0.03936
0.03740
                         D83       D84
          1             -0.04602  -0.04146
 RFO step:  Lambda0=5.020651195D-09 Lambda=-4.33076982D-07.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.00063876 RMS(Int)=  0.00000021
 Iteration  2 RMS(Cart)=  0.00000028 RMS(Int)=  0.00000007
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.74745  -0.00006   0.00000   0.00007   0.00007
2.74751
    R2        2.68850  -0.00002   0.00000  -0.00005  -0.00005
2.68845
    R3        5.52118  -0.00002   0.00000  -0.00232  -0.00232
5.51886
    R4        2.67717  -0.00002   0.00000  -0.00006  -0.00006
2.67711
    R5        4.55166  -0.00001   0.00000  -0.00408  -0.00408
4.54758
    R6        4.94541  -0.00002   0.00000  -0.00351  -0.00351
4.94190
    R7        2.75059   0.00002   0.00000   0.00023   0.00023
2.75082
    R8        2.81837   0.00001   0.00000   0.00020   0.00020
2.81856
    R9        2.73033   0.00000   0.00000  -0.00017  -0.00017
2.73016
   R10        5.19662   0.00001   0.00000   0.00115   0.00115
5.19777
   R11        2.66471   0.00000   0.00000   0.00004   0.00004
2.66475
   R12        2.05759   0.00000   0.00000  -0.00001  -0.00001
2.05757
   R13        3.87505   0.00002   0.00000   0.00219   0.00219
3.87724
   R14        4.51620   0.00001   0.00000   0.00148   0.00148
4.51769
   R15        2.73661  -0.00002   0.00000  -0.00017  -0.00017
2.73644
   R16        4.69172   0.00000   0.00000   0.00189   0.00189
4.69361
```

This journal is © The Royal Society of Chemistry 2014

R17	2.04814	-0.00001	0.00000	-0.00004	-0.00004
2.04809					
R18	2.67026	-0.00002	0.00000	-0.00006	-0.00006
2.67020					
R19	5.03526	0.00000	0.00000	0.00058	0.00058
5.03584					
R20	2.82425	0.00000	0.00000	-0.00024	-0.00024
2.82401					
R21	5.13357	-0.00001	0.00000	-0.00024	-0.00024
5.13332					
R22	2.04291	0.00001	0.00000	0.00002	0.00002
2.04293					
R23	5.40657	-0.00001	0.00000	-0.00231	-0.00231
5.40426					
R24	2.78441	0.00000	0.00000	0.00024	0.00024
2.78465					
R25	5.37590	-0.00001	0.00000	-0.00177	-0.00177
5.37413					
R26	5.36028	0.00000	0.00000	-0.00290	-0.00290
5.35738					
R27	2.04963	0.00001	0.00000	0.00000	0.00000
2.04963					
R28	2.61809	0.00000	0.00000	0.00002	0.00002
2.61810					
R29	2.05319	0.00000	0.00000	0.00000	0.00000
2.05319					
R30	2.66281	0.00001	0.00000	0.00000	0.00000
2.66280					
R31	2.05281	0.00000	0.00000	0.00000	0.00000
2.05282					
R32	2.61672	0.00001	0.00000	-0.00001	-0.00001
2.61671					
R33	2.05361	0.00000	0.00000	0.00000	0.00000
2.05361					
R34	2.68948	0.00000	0.00000	0.00003	0.00003
2.68951					
R35	2.66241	0.00000	0.00000	0.00004	0.00004
2.66245					
R36	2.67674	0.00004	0.00000	0.00007	0.00007
2.67681					
R37	2.04385	-0.00001	0.00000	-0.00005	-0.00005
2.04380					
R38	2.62149	-0.00001	0.00000	-0.00001	-0.00001
2.62148					
R39	4.19510	0.00004	0.00000	0.00024	0.00024
4.19533					
R40	2.05368	0.00000	0.00000	0.00000	0.00000
2.05368					
R41	2.66181	0.00000	0.00000	-0.00003	-0.00003
2.66178					
R42	2.05358	0.00000	0.00000	0.00000	0.00000
2.05358					

This journal is © The Royal Society of Chemistry 2014

R43	2.61919	-0.00001	0.00000	-0.00006	-0.00006
2.61913					
R44	2.05542	0.00000	0.00000	0.00000	0.00000
2.05541					
R45	2.65933	0.00000	0.00000	-0.00022	-0.00022
2.65911					
R46	2.27420	0.00000	0.00000	-0.00001	-0.00001
2.27419					
R47	2.62221	-0.00001	0.00000	0.00016	0.00016
2.62237					
R48	2.27259	0.00000	0.00000	0.00000	0.00000
2.27259					
R49	2.08475	0.00002	0.00000	0.00003	0.00003
2.08478					
R50	2.30654	-0.00003	0.00000	-0.00007	-0.00007
2.30648					
A1	2.04072	0.00000	0.00000	-0.00004	-0.00004
2.04068					
A2	2.17374	-0.00003	0.00000	-0.00001	-0.00001
2.17372					
A3	2.06845	0.00003	0.00000	0.00004	0.00004
2.06849					
A4	2.05299	0.00001	0.00000	-0.00014	-0.00014
2.05285					
A5	2.05955	-0.00002	0.00000	-0.00016	-0.00016
2.05939					
A6	2.13586	0.00000	0.00000	-0.00007	-0.00007
2.13580					
A7	2.03301	0.00000	0.00000	-0.00001	-0.00001
2.03300					
A8	2.10007	-0.00002	0.00000	-0.00003	-0.00003
2.10005					
A9	2.14737	0.00002	0.00000	0.00004	0.00004
2.14742					
A10	2.03886	0.00000	0.00000	0.00019	0.00019
2.03905					
A11	2.04240	0.00000	0.00000	0.00015	0.00015
2.04254					
A12	2.04673	0.00000	0.00000	0.00018	0.00018
2.04691					
A13	2.15510	0.00001	0.00000	0.00033	0.00033
2.15543					
A14	2.05475	-0.00001	0.00000	0.00022	0.00022
2.05497					
A15	1.85375	0.00001	0.00000	0.00020	0.00020
1.85395					
A16	2.20990	0.00001	0.00000	-0.00011	-0.00011
2.20979					
A17	1.87926	-0.00001	0.00000	-0.00019	-0.00019
1.87908					
A18	2.10113	-0.00001	0.00000	-0.00022	-0.00022
2.10091					

A19	2.10386	-0.00001	0.00000	-0.00003	-0.00003
2.10383					
A20	2.09942	-0.00001	0.00000	-0.00001	-0.00001
2.09941					
A21	2.07928	0.00002	0.00000	0.00005	0.00005
2.07932					
A22	2.08531	0.00000	0.00000	0.00001	0.00001
2.08532					
A23	2.10836	-0.00001	0.00000	-0.00001	-0.00001
2.10835					
A24	2.08951	0.00000	0.00000	0.00000	0.00000
2.08952					
A25	2.09276	0.00000	0.00000	0.00000	0.00000
2.09276					
A26	2.09468	0.00001	0.00000	0.00001	0.00001
2.09468					
A27	2.09575	0.00000	0.00000	0.00000	0.00000
2.09574					
A28	2.09462	0.00000	0.00000	-0.00001	-0.00001
2.09461					
A29	2.08278	0.00000	0.00000	0.00000	0.00000
2.08278					
A30	2.10571	0.00000	0.00000	0.00000	0.00000
2.10571					
A31	2.04123	-0.00001	0.00000	0.00000	0.00000
2.04124					
A32	2.13707	0.00001	0.00000	-0.00004	-0.00004
2.13703					
A33	2.10078	0.00000	0.00000	0.00005	0.00005
2.10082					
A34	2.03024	-0.00001	0.00000	-0.00011	-0.00011
2.03013					
A35	2.18240	0.00001	0.00000	0.00021	0.00021
2.18261					
A36	2.06949	-0.00001	0.00000	-0.00010	-0.00010
2.06939					
A37	2.08494	-0.00001	0.00000	0.00011	0.00011
2.08506					
A38	2.09602	0.00000	0.00000	0.00004	0.00004
2.09606					
A39	2.10215	0.00001	0.00000	-0.00016	-0.00016
2.10199					
A40	2.08294	0.00001	0.00000	0.00000	0.00000
2.08294					
A41	2.11173	0.00000	0.00000	0.00001	0.00001
2.11174					
A42	2.08851	0.00000	0.00000	-0.00001	-0.00001
2.08850					
A43	2.09499	-0.00001	0.00000	0.00000	0.00000
2.09499					
A44	2.09200	0.00001	0.00000	-0.00001	-0.00001
2.09199					

A45	2.09620	-0.00001	0.00000	0.00001	0.00001	2.09621
A46	2.09545	0.00000	0.00000	0.00001	0.00001	2.09545
A47	2.08318	0.00000	0.00000	-0.00001	-0.00001	2.08316
A48	2.10431	0.00000	0.00000	0.00000	0.00000	2.10432
A49	1.88315	0.00001	0.00000	0.00006	0.00006	1.88322
A50	2.28832	0.00000	0.00000	-0.00014	-0.00014	2.28817
A51	2.11171	-0.00001	0.00000	0.00008	0.00008	2.11179
A52	1.88821	0.00000	0.00000	-0.00004	-0.00004	1.88817
A53	2.26109	0.00000	0.00000	0.00013	0.00013	2.26122
A54	2.13366	0.00000	0.00000	-0.00009	-0.00009	2.13357
A55	1.90744	0.00000	0.00000	-0.00001	-0.00001	1.90742
A56	2.00149	0.00001	0.00000	0.00012	0.00012	2.00161
A57	2.19151	-0.00002	0.00000	-0.00003	-0.00003	2.19148
A58	2.08875	0.00001	0.00000	-0.00008	-0.00008	2.08867
D1	-0.56812	0.00000	0.00000	-0.00054	-0.00054	-0.56866
D2	2.84682	0.00001	0.00000	0.00088	0.00088	2.84771
D3	2.59934	0.00000	0.00000	-0.00019	-0.00019	2.59915
D4	-0.26890	0.00001	0.00000	0.00123	0.00123	-0.26767
D5	-0.02919	0.00000	0.00000	0.00049	0.00049	-0.02869
D6	-3.09387	0.00000	0.00000	0.00036	0.00036	-3.09352
D7	3.08816	0.00000	0.00000	0.00017	0.00017	3.08832
D8	0.02347	0.00000	0.00000	0.00003	0.00003	0.02350
D9	-0.05509	0.00000	0.00000	-0.00023	-0.00023	-0.05532
D10	3.12503	0.00000	0.00000	-0.00033	-0.00033	3.12470
D11	3.11276	0.00000	0.00000	0.00012	0.00012	3.11288
D12	0.00969	0.00000	0.00000	0.00002	0.00002	0.00971

This journal is © The Royal Society of Chemistry 2014

D13	0.56060	0.00000	0.00000	0.00036	0.00036	0.56096
D14	-2.63115	0.00000	0.00000	0.00018	0.00018	-2.63097
D15	-2.86710	-0.00002	0.00000	-0.00114	-0.00114	-2.86825
D16	0.22434	-0.00002	0.00000	-0.00132	-0.00132	0.22301
D17	-0.37659	0.00001	0.00000	-0.00015	-0.00015	-0.37674
D18	2.82311	-0.00004	0.00000	-0.00045	-0.00045	2.82267
D19	3.05213	0.00002	0.00000	0.00136	0.00136	3.05349
D20	-0.03135	-0.00003	0.00000	0.00106	0.00106	-0.03029
D21	-3.09461	0.00001	0.00000	0.00074	0.00074	-3.09387
D22	0.63128	0.00000	0.00000	-0.00021	-0.00021	0.63108
D23	-0.03220	0.00001	0.00000	0.00087	0.00087	-0.03133
D24	-2.58950	0.00000	0.00000	-0.00007	-0.00007	-2.58957
D25	-0.04150	0.00000	0.00000	-0.00005	-0.00005	-0.04154
D26	3.11394	0.00000	0.00000	0.00000	0.00000	3.11394
D27	-3.10097	0.00000	0.00000	-0.00019	-0.00019	-3.10116
D28	0.05447	0.00000	0.00000	-0.00014	-0.00014	0.05433
D29	-0.63851	0.00000	0.00000	0.00005	0.00005	-0.63845
D30	2.60014	0.00000	0.00000	-0.00003	-0.00003	2.60011
D31	3.09005	-0.00001	0.00000	-0.00090	-0.00090	3.08915
D32	0.04551	0.00000	0.00000	-0.00099	-0.00099	0.04452
D33	-0.17163	0.00000	0.00000	0.00180	0.00180	-0.16983
D34	2.51488	0.00000	0.00000	0.00054	0.00054	2.51542
D35	-2.62633	0.00000	0.00000	0.00072	0.00072	-2.62561
D36	0.06018	0.00000	0.00000	-0.00054	-0.00054	0.05964
D37	-2.63510	-0.00001	0.00000	-0.00066	-0.00066	-2.63576
D38	0.52920	-0.00001	0.00000	-0.00071	-0.00071	0.52849

This journal is © The Royal Society of Chemistry 2014

D39	-0.13396	0.00000	0.00000	0.00040	0.00040	-0.13356
D40	3.03034	0.00000	0.00000	0.00035	0.00035	3.03069
D41	0.03173	0.00000	0.00000	0.00051	0.00051	0.03224
D42	-3.10771	0.00000	0.00000	0.00037	0.00037	-3.10734
D43	2.75201	0.00001	0.00000	-0.00062	-0.00062	2.75139
D44	-0.38743	0.00000	0.00000	-0.00075	-0.00075	-0.38818
D45	3.11581	0.00000	0.00000	-0.00001	-0.00001	3.11580
D46	-0.02529	0.00000	0.00000	-0.00006	-0.00006	-0.02535
D47	0.01220	0.00000	0.00000	-0.00010	-0.00010	0.01210
D48	-3.12889	0.00000	0.00000	-0.00015	-0.00015	-3.12905
D49	-3.13273	0.00000	0.00000	0.00006	0.00006	-3.13267
D50	0.00734	0.00000	0.00000	0.00004	0.00004	0.00739
D51	0.00936	0.00000	0.00000	0.00001	0.00001	0.00937
D52	-3.13375	0.00000	0.00000	-0.00001	-0.00001	-3.13376
D53	0.02606	0.00000	0.00000	0.00001	0.00001	0.02607
D54	-3.12956	0.00000	0.00000	-0.00004	-0.00004	-3.12960
D55	-3.11705	0.00000	0.00000	-0.00001	-0.00001	-3.11706
D56	0.01051	0.00000	0.00000	-0.00006	-0.00006	0.01045
D57	0.03950	0.00001	0.00000	-0.00018	-0.00018	0.03932
D58	-3.05534	0.00001	0.00000	-0.00002	-0.00002	-3.05536
D59	3.08617	0.00000	0.00000	-0.00010	-0.00010	3.08607
D60	-0.00867	0.00000	0.00000	0.00006	0.00006	-0.00861
D61	3.07870	0.00000	0.00000	0.00009	0.00009	3.07880
D62	-0.08680	0.00000	0.00000	0.00008	0.00008	-0.08671
D63	0.03738	0.00000	0.00000	0.00001	0.00001	0.03739
D64	-3.12812	0.00000	0.00000	0.00000	0.00000	-3.12812

```
   D65        0.03821  -0.00001   0.00000   0.00010   0.00010
0.03831
   D66       -3.11656   0.00000   0.00000   0.00010   0.00010  -
3.11646
   D67        3.12862  -0.00001   0.00000  -0.00009  -0.00009
3.12853
   D68       -0.02616   0.00000   0.00000  -0.00008  -0.00008  -
0.02624
   D69       -3.10943   0.00000   0.00000   0.00001   0.00001  -
3.10942
   D70        0.03296   0.00000   0.00000   0.00004   0.00004
0.03300
   D71        0.01885   0.00001   0.00000   0.00002   0.00002
0.01887
   D72       -3.12195   0.00001   0.00000   0.00005   0.00005  -
3.12189
   D73        3.13915   0.00000   0.00000  -0.00001  -0.00001
3.13914
   D74       -0.00407   0.00000   0.00000   0.00002   0.00002  -
0.00405
   D75       -0.00164   0.00000   0.00000   0.00002   0.00002  -
0.00161
   D76        3.13832   0.00000   0.00000   0.00006   0.00006
3.13838
   D77       -0.03109   0.00000   0.00000  -0.00004  -0.00004  -
0.03113
   D78        3.13471   0.00000   0.00000  -0.00004  -0.00004
3.13467
   D79        3.10887   0.00000   0.00000  -0.00001  -0.00001
3.10886
   D80       -0.00852   0.00000   0.00000  -0.00001  -0.00001  -
0.00853
   D81       -0.11893   0.00000   0.00000  -0.00024  -0.00024  -
0.11917
   D82        3.02077   0.00000   0.00000  -0.00012  -0.00012
3.02065
   D83        0.15660   0.00000   0.00000  -0.00010  -0.00010
0.15651
   D84       -3.00569   0.00000   0.00000  -0.00004  -0.00004  -
3.00573
         Item               Value     Threshold  Converged?
 Maximum Force            0.000056     0.000450     YES
 RMS     Force            0.000011     0.000300     YES
 Maximum Displacement     0.002614     0.001800     NO
 RMS     Displacement     0.000639     0.001200     YES
 Predicted change in Energy=-2.140277D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.556075	0.522868	1.163163
2	6	0	0.604289	1.084962	0.491230
3	6	0	-0.741529	-0.883879	1.059947
4	6	0	0.225761	-1.604598	0.264844
5	1	0	0.063403	-2.674462	0.144175
6	6	0	-0.203462	-0.963387	-1.636281
7	1	0	0.492507	-1.645552	-2.110531
8	6	0	-0.096185	0.443068	-1.719752
9	1	0	0.737494	1.003516	-2.119247
10	6	0	-1.516068	1.280965	1.877756
11	1	0	-1.393193	2.351696	1.999539
12	6	0	-2.601380	0.654950	2.469066
13	1	0	-3.316745	1.245834	3.034393
14	6	0	-2.786866	-0.736456	2.346050
15	1	0	-3.647531	-1.211116	2.808658
16	6	0	-1.873936	-1.496780	1.634803
17	1	0	-2.012853	-2.568884	1.524055
18	6	0	1.597348	-1.143489	0.319755
19	6	0	1.802289	0.261925	0.411331
20	6	0	3.128152	0.757863	0.360174
21	1	0	3.299811	1.824214	0.416217
22	6	0	4.196091	-0.121242	0.254888
23	1	0	5.209700	0.270653	0.246975
24	6	0	3.985074	-1.510482	0.157402
25	1	0	4.833056	-2.184857	0.073279
26	6	0	2.694273	-2.015060	0.170939
27	1	0	2.517822	-3.085266	0.089892
28	6	0	-1.461969	0.992711	-1.782557
29	6	0	-1.661208	-1.277458	-1.734097
30	8	0	-2.365389	-0.082405	-1.693109
31	8	0	-2.211338	-2.344007	-1.812048
32	8	0	-1.854893	2.125010	-1.891158
33	6	0	0.628907	2.556637	0.249987
34	1	0	-0.362128	3.041288	0.256969
35	8	0	1.623236	3.218150	-0.001838

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.453921	0.000000			
3	C	1.422667	2.451734	0.000000		
4	C	2.438104	2.725485	1.444741	0.000000	
5	H	3.412477	3.813957	2.166274	1.088820	0.000000
6	C	3.189072	3.061781	2.750543	2.051746	2.483751
7	H	4.064313	3.773243	3.486392	2.390656	2.515251
8	C	2.920456	2.406477	3.147060	2.869705	3.635751
9	H	3.560696	2.615143	3.982090	3.570437	4.370926
10	C	1.416666	2.541019	2.440342	3.736566	4.598416
11	H	2.178281	2.805270	3.431682	4.613290	5.552145

This journal is © The Royal Society of Chemistry 2014

12	C	2.430248	3.791181	2.795113	4.237556	4.857074
13	H	3.412548	4.676330	3.881475	5.323976	5.928531
14	C	2.821621	4.272920	2.420577	3.763111	4.090006
15	H	3.907872	5.359143	3.407334	4.650614	4.797070
16	C	2.457271	3.756960	1.410125	2.509410	2.713335
17	H	3.436768	4.611588	2.161227	2.743511	2.495206
18	C	2.850493	2.445724	2.466907	1.448063	2.174326
19	C	2.489020	1.455671	2.864364	2.447613	3.423078
20	C	3.778034	2.548344	4.261389	3.743553	4.606539
21	H	4.137546	2.796062	4.907197	4.607543	5.548552
22	C	4.880873	3.796292	5.060616	4.238392	4.859043
23	H	5.843557	4.683222	6.116452	5.325085	5.930315
24	C	5.076228	4.275217	4.852627	3.762025	4.090785
25	H	6.128812	5.361797	5.808791	4.647641	4.795240
26	C	4.241503	3.752434	3.724868	2.504167	2.712380
27	H	4.859977	4.605810	4.050986	2.734325	2.489153
28	C	3.117477	3.073766	3.481444	3.712990	4.414432
29	C	3.585611	3.957977	2.967726	2.768291	2.907544
30	O	3.434860	3.866920	3.295239	3.586741	3.999175
31	O	4.450927	4.999067	3.541281	3.286283	3.018353
32	O	3.685467	3.578415	4.359130	4.784082	5.554941
33	C	2.524736	1.491520	3.790947	4.180745	5.262641
34	H	2.683513	2.194550	4.024382	4.682940	5.732677
35	O	3.656661	2.414925	4.852437	5.028216	6.097317

		6	7	8	9	10
6	C	0.000000				
7	H	1.083805	0.000000			
8	C	1.413008	2.204903	0.000000		
9	H	2.233240	2.660386	1.081073	0.000000	
10	C	4.371328	5.339036	3.957297	4.596906	0.000000
11	H	5.062058	6.035440	4.377010	4.829267	1.084617
12	C	5.022241	5.986415	4.885396	5.685261	1.385441
13	H	6.032279	7.024298	5.798132	6.561675	2.140440
14	C	4.752308	5.607303	5.016152	5.948738	2.429859
15	H	5.628541	6.444151	5.987895	6.958253	3.408840
16	C	3.711467	4.432800	4.263384	5.211903	2.811221
17	H	3.979855	4.509943	4.823666	5.796559	3.897851
18	C	2.664851	2.716438	3.089467	3.361207	4.242487
19	C	3.117233	3.422541	2.859813	2.843865	3.768333
20	C	4.248316	4.339057	3.849875	3.452988	4.913804
21	H	4.925078	5.128810	4.242961	3.696971	5.062006
22	C	4.862283	4.651372	4.758285	4.343212	6.101528
23	H	5.862749	5.610846	5.661285	5.112409	6.994006
24	C	4.589166	4.166508	4.898646	4.695752	6.404244
25	H	5.457206	4.888788	5.866717	5.634405	7.455161
26	C	3.573364	3.192087	4.171782	4.264474	5.612840
27	H	3.858423	3.319118	4.749419	4.976746	6.207471
28	C	2.330570	3.299693	1.473573	2.225109	3.672043
29	C	1.494401	2.217134	2.325879	3.332409	4.428552
30	O	2.335228	3.284089	2.329403	3.314921	3.915508
31	O	2.443066	2.808507	3.500026	4.471677	5.219049
32	O	3.511465	4.446971	2.439542	2.833768	3.877103

33	C	4.079390	4.821727	2.978726	2.835005	2.979578
34	H	4.432493	5.319955	3.275499	3.317843	2.656551
35	O	4.847008	5.420400	3.688999	3.189446	4.140143
		11	12	13	14	15
11	H	0.000000				
12	C	2.135209	0.000000			
13	H	2.448246	1.086501	0.000000		
14	C	3.405742	1.409096	2.164270	0.000000	
15	H	4.293058	2.166093	2.489373	1.086303	0.000000
16	C	3.895500	2.419735	3.400366	1.384704	2.145969
17	H	4.982186	3.410648	4.305035	2.152339	2.483125
18	C	4.897073	5.048093	6.101347	4.846945	5.805857
19	C	4.135294	4.876581	5.835499	5.079394	6.133317
20	C	5.066595	6.106190	6.994732	6.415928	7.468724
21	H	4.980907	6.356526	7.139201	6.879602	7.950005
22	C	6.356046	7.191014	8.126331	7.315267	8.320576
23	H	7.141457	8.130088	9.023355	8.328591	9.338544
24	C	6.872819	7.308506	8.318108	7.158802	8.085508
25	H	7.940841	8.311145	9.325079	8.082484	8.963862
26	C	6.254576	6.360368	7.413848	6.033972	6.915372
27	H	6.964434	6.771700	7.840325	6.224698	6.993977
28	C	4.019430	4.414593	5.167908	4.668058	5.541912
29	C	5.213696	4.720667	5.643252	4.267011	4.958478
30	O	4.528318	4.233566	5.001857	4.113420	4.814954
31	O	6.103048	5.241547	6.131629	4.495022	4.969609
32	O	3.924548	4.661531	5.212583	5.197162	6.035857
33	C	2.681757	4.356085	5.003928	5.187046	6.247455
34	H	2.138968	3.949966	4.434806	4.951259	5.948776
35	O	3.722243	5.524739	6.124716	6.371851	7.436281
		16	17	18	19	20
16	C	0.000000				
17	H	1.086724	0.000000			
18	C	3.728803	4.063944	0.000000		
19	C	4.254945	4.879236	1.423227	0.000000	
20	C	5.632848	6.233121	2.441339	1.416505	0.000000
21	H	6.267504	6.982193	3.422711	2.164103	1.081532
22	C	6.375068	6.793580	2.793325	2.429317	1.387229
23	H	7.431539	7.865060	3.879972	3.411383	2.140800
24	C	6.042424	6.242041	2.421214	2.823199	2.433273
25	H	6.920660	7.008473	3.408079	3.909804	3.413005
26	C	4.824940	4.928963	1.408910	2.457251	2.813035
27	H	4.919103	4.780219	2.161159	3.437877	3.900666
28	C	4.248015	4.891024	4.282813	4.000321	5.071061
29	C	3.382727	3.522356	3.854146	4.355270	5.609499
30	O	3.649244	4.081299	4.569552	4.681535	5.924612
31	O	3.565447	3.349560	4.526800	5.276694	6.546015
32	O	5.054714	5.807002	5.243014	4.706116	5.636340
33	C	4.961061	5.905346	3.825399	2.582355	3.081226
34	H	4.977756	5.983680	4.621238	3.526101	4.172138
35	O	6.094208	7.002803	4.373555	2.990323	2.906688
		21	22	23	24	25
21	H	0.000000				

This journal is © The Royal Society of Chemistry 2014

22	C	2.148056	0.000000			
23	H	2.467766	1.086760	0.000000		
24	C	3.414200	1.408552	2.163371	0.000000	
25	H	4.305937	2.167305	2.490293	1.086707	0.000000
26	C	3.894465	2.418481	3.399652	1.385983	2.147733
27	H	4.982066	3.410168	4.305005	2.153446	2.484214
28	C	5.310419	6.116021	7.010815	6.300769	7.291666
29	C	6.233453	6.292921	7.316466	5.959242	6.801871
30	O	6.338687	6.844649	7.827551	6.766991	7.704417
31	O	7.260303	7.089997	8.133132	6.555076	7.294057
32	O	5.655567	6.801880	7.610435	7.177647	8.195281
33	C	2.774492	4.460478	5.119511	5.273887	6.339389
34	H	3.862179	5.547879	6.222682	6.294973	7.371313
35	O	2.220075	4.223391	4.648910	5.288061	6.284987

		26	27	28	29	30
26	C	0.000000				
27	H	1.087678	0.000000			
28	C	5.489734	5.997891	0.000000		
29	C	4.810763	4.905039	2.279410	0.000000	
30	O	5.728003	6.003501	1.407141	1.387696	0.000000
31	O	5.301459	5.150903	3.419958	1.202600	2.269961
32	O	6.487476	7.084644	1.203447	3.411593	2.274316
33	C	5.017210	5.951865	3.308907	4.886871	4.439142
34	H	5.908946	6.771756	3.092892	4.929859	4.192054
35	O	5.344479	6.367240	4.200241	5.830848	5.446393

		31	32	33	34	35
31	O	0.000000				
32	O	4.483908	0.000000			
33	C	6.027877	3.307578	0.000000		
34	H	6.058202	2.771708	1.103216	0.000000	
35	O	6.994170	4.106321	1.220535	2.009958	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.521058	0.690433	1.079516
2	6	0	0.627322	1.131757	0.304698
3	6	0	-0.724139	-0.713509	1.187616
4	6	0	0.214347	-1.556336	0.483227
5	1	0	0.037492	-2.629914	0.524251
6	6	0	-0.257435	-1.193251	-1.480253
7	1	0	0.418614	-1.947232	-1.866393
8	6	0	-0.137371	0.184291	-1.771040
9	1	0	0.691540	0.668425	-2.268271
10	6	0	-1.453950	1.558384	1.698642

```
   11          1               0       -1.316524    2.633549    1.659550
   12          6               0       -2.530093    1.040990    2.401255
   13          1               0       -3.224129    1.718242    2.891283
   14          6               0       -2.733557   -0.350667    2.487531
   15          1               0       -3.586883   -0.740345    3.035290
   16          6               0       -1.847646   -1.219656    1.873181
   17          1               0       -2.000834   -2.294339    1.923775
   18          6               0        1.591740   -1.111899    0.436871
   19          6               0        1.813982    0.288748    0.316983
   20          6               0        3.143277    0.752821    0.161747
   21          1               0        3.327706    1.813361    0.057099
   22          6               0        4.198667   -0.147487    0.160275
   23          1               0        5.215848    0.224461    0.070585
   24          6               0        3.970370   -1.532909    0.272102
   25          1               0        4.808627   -2.224451    0.266957
   26          6               0        2.675051   -2.011520    0.390547
   27          1               0        2.485139   -3.079453    0.471147
   28          6               0       -1.498386    0.738450   -1.880414
   29          6               0       -1.720504   -1.497260   -1.495738
   30          8               0       -2.410586   -0.299025   -1.612865
   31          8               0       -2.283827   -2.555758   -1.403555
   32          8               0       -1.881906    1.848315   -2.143847
   33          6               0        0.661342    2.551983   -0.149652
   34          1               0       -0.323947    3.046650   -0.189590
   35          8               0        1.655768    3.155327   -0.519514
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3890152      0.2596750
0.2420823
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1906.9514892716 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

Supplementary Material (ESI) for Green Chemistry
This journal is © The Royal Society of Chemistry 2014

```
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                  (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1032.13801888     A.U. after   12 cycles
             Convg  =    0.6266D-08             -V/T =  2.0093
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.000000308    0.000007650   -0.000017127
    2          6          -0.000006087    0.000003586    0.000010343
    3          6           0.000003083   -0.000005702   -0.000006570
    4          6           0.000007484   -0.000000598    0.000010266
    5          1           0.000001803    0.000000364   -0.000001074
    6          6           0.000004516    0.000018831   -0.000009797
    7          1           0.000000038    0.000000612   -0.000001305
    8          6          -0.000004167   -0.000014559    0.000000197
```

9	1	0.000002359	0.000007226	0.000020056
10	6	-0.000000315	-0.000001168	0.000004035
11	1	0.000003890	0.000001898	0.000002892
12	6	0.000000191	-0.000001923	-0.000001134
13	1	-0.000000903	-0.000003813	0.000000659
14	6	0.000001588	-0.000003806	-0.000000593
15	1	0.000000689	-0.000003724	-0.000000646
16	6	0.000000670	-0.000001769	-0.000000294
17	1	0.000001565	-0.000002158	-0.000001842
18	6	-0.000005722	-0.000005539	0.000000644
19	6	-0.000013847	0.000003449	-0.000009404
20	6	0.000014373	-0.000001674	0.000006441
21	1	0.000005880	-0.000004161	-0.000005497
22	6	-0.000001375	0.000003273	0.000000211
23	1	-0.000000057	0.000002876	0.000001015
24	6	-0.000002485	0.000002902	-0.000000964
25	1	0.000001347	0.000003230	-0.000000864
26	6	0.000005642	0.000001723	-0.000000128
27	1	0.000002505	0.000001565	-0.000001334
28	6	0.000002251	0.000001411	0.000002849
29	6	-0.000002469	0.000001390	0.000000578
30	8	0.000000929	-0.000002342	0.000003102
31	8	0.000002596	0.000000321	-0.000000391
32	8	-0.000003130	-0.000002119	-0.000001778
33	6	0.000003927	-0.000016491	-0.000021995
34	1	-0.000012288	-0.000003258	0.000003953
35	8	-0.000014787	0.000012498	0.000015495

Cartesian Forces: Max 0.000021995 RMS 0.000006508

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Internal Forces: Max 0.000018169 RMS 0.000004101
Search for a saddle point.
Step number 10 out of a maximum of 202
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Swaping is turned off.
Update second derivatives using D2CorX and points 4 5 6 7 8
9 10
Eigenvalues --- -0.01889 0.00247 0.00397 0.00757
0.00855
Eigenvalues --- 0.01044 0.01265 0.01445 0.01486
0.01539
Eigenvalues --- 0.01643 0.01680 0.01775 0.01884
0.01931
Eigenvalues --- 0.01996 0.02127 0.02174 0.02189
0.02238
Eigenvalues --- 0.02362 0.02428 0.02449 0.02522
0.02665

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02717   0.02746   0.02749   0.03072
0.03506
     Eigenvalues ---    0.04004   0.05546   0.07030   0.07399
0.07487
     Eigenvalues ---    0.08785   0.10176   0.11043   0.11179
0.11222
     Eigenvalues ---    0.11859   0.12278   0.12499   0.12527
0.12658
     Eigenvalues ---    0.12832   0.13903   0.14258   0.14660
0.16395
     Eigenvalues ---    0.17651   0.18500   0.19087   0.19170
0.19333
     Eigenvalues ---    0.19414   0.20109   0.20401   0.20899
0.21163
     Eigenvalues ---    0.23351   0.23905   0.24400   0.25102
0.26061
     Eigenvalues ---    0.27638   0.27927   0.29099   0.30147
0.30310
     Eigenvalues ---    0.31232   0.33071   0.33988   0.34005
0.35001
     Eigenvalues ---    0.35273   0.35918   0.36086   0.36133
0.36201
     Eigenvalues ---    0.36237   0.36329   0.36534   0.37397
0.37810
     Eigenvalues ---    0.38852   0.39855   0.40317   0.41115
0.42458
     Eigenvalues ---    0.44479   0.46263   0.47304   0.47636
0.50256
     Eigenvalues ---    0.50616   0.79373   0.89039
0.902561000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                          R1        R2        R3        R4        R5
          1             -0.04225   0.02310   0.14381   0.01761
0.34982
                          R6        R7        R8        R9        R10
          1              0.08805  -0.04257  -0.01978  -0.06215
0.19929
                          R11       R12       R13       R14       R15
          1              0.01928  -0.00709   0.45650   0.19237  -
0.05999
                          R16       R17       R18       R19       R20
          1              0.30425  -0.00770  -0.09441   0.18923  -
0.01460
                          R21       R22       R23       R24       R25
          1             -0.02929  -0.00690   0.14649  -0.00461  -
0.04609
                          R26       R27       R28       R29       R30
          1              0.05874  -0.00130  -0.01344   0.00008
0.01444
                          R31       R32       R33       R34       R35
          1             -0.00024  -0.01608  -0.00024   0.02114
0.01855
                          R36       R37       R38       R39       R40
          1              0.01788  -0.00159  -0.01221  -0.04862
0.00008
                          R41       R42       R43       R44       R45
          1              0.01313  -0.00013  -0.01566  -0.00014
0.00128
                          R46       R47       R48       R49       R50
          1              0.00079  -0.00065   0.00267  -0.00118
0.00469
                          A1        A2        A3        A4        A5
          1              0.02098  -0.00775  -0.01312   0.03161  -
0.00488
                          A6        A7        A8        A9        A10
          1              0.00708   0.01909  -0.00141  -0.01644
0.03387
```

This journal is © The Royal Society of Chemistry 2014

	A11	A12	A13	A14	A15
1	0.05786	0.03058	0.06391	0.04380	0.02361
	A16	A17	A18	A19	A20
1	0.04597	0.00633	0.01523	-0.00377	0.00674
	A21	A22	A23	A24	A25
1	-0.00306	-0.00133	0.00487	-0.00353	-0.00137
	A26	A27	A28	A29	A30
1	-0.00132	0.00270	0.00408	-0.00661	0.00245
	A31	A32	A33	A34	A35
1	0.01964	-0.01819	-0.00049	0.02073	-0.00694
	A36	A37	A38	A39	A40
1	-0.01381	-0.00321	0.00710	-0.00390	-0.00110
	A41	A42	A43	A44	A45
1	0.00451	-0.00341	-0.00109	-0.00156	0.00265
	A46	A47	A48	A49	A50
1	0.00424	-0.00639	0.00206	-0.00221	0.00133
	A51	A52	A53	A54	A55
1	0.00087	-0.00680	0.00481	0.00210	-0.01368
	A56	A57	A58	D1	D2
1	-0.00158	0.00963	-0.00807	0.12973	-0.00044
	D3	D4	D5	D6	D7
1	0.12515	-0.00503	0.02331	0.00642	0.02765
	D8	D9	D10	D11	D12
1	0.01076	-0.00533	-0.00252	-0.01046	-0.00765
	D13	D14	D15	D16	D17
1	-0.13454	-0.13532	-0.00003	-0.00082	0.07916
	D18	D19	D20	D21	D22
1	0.07978	-0.06153	-0.06091	0.05523	-0.16204
	D23	D24	D25	D26	D27
1	0.07340	-0.14386	-0.00626	0.00046	-0.02596
	D28	D29	D30	D31	D32
1	-0.01925	0.15707	0.14561	-0.06236	-0.07382
	D33	D34	D35	D36	D37
1	0.02433	0.18088	-0.16623	-0.00968	-0.15493
	D38	D39	D40	D41	D42

```
          1             -0.16005   0.03255   0.02743  -0.01557  -
0.01372
                           D43       D44       D45       D46       D47
          1              0.13912   0.14097  -0.00126  -0.00036
0.00153
                           D48       D49       D50       D51       D52
          1              0.00242   0.00063   0.00515   0.00153
0.00605
                           D53       D54       D55       D56       D57
          1             -0.00177  -0.00865   0.00275  -0.00412  -
0.01322
                           D58       D59       D60       D61       D62
          1             -0.01262  -0.00309  -0.00248   0.01414
0.00993
                           D63       D64       D65       D66       D67
          1              0.00126  -0.00295   0.00239   0.00147
0.00250
                           D68       D69       D70       D71       D72
          1              0.00158   0.00211   0.00088   0.00119  -
0.00004
                           D73       D74       D75       D76       D77
          1              0.00096  -0.00201  -0.00027  -0.00324
0.00096
                           D78       D79       D80       D81       D82
          1              0.00534  -0.00202   0.00236   0.03845
0.03683
                           D83       D84
          1             -0.04640  -0.04167
 RFO step:  Lambda0=2.376294321D-09 Lambda=-8.64877237D-08.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.00032675 RMS(Int)=  0.00000021
 Iteration  2 RMS(Cart)=  0.00000026 RMS(Int)=  0.00000005
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.74751  -0.00002   0.00000  -0.00001  -0.00001
2.74751
    R2        2.68845   0.00000   0.00000  -0.00002  -0.00002
2.68843
    R3        5.51886  -0.00001   0.00000  -0.00067  -0.00067
5.51819
    R4        2.67711   0.00000   0.00000  -0.00001  -0.00001
2.67710
    R5        4.54758   0.00000   0.00000  -0.00100  -0.00100
4.54658
    R6        4.94190   0.00000   0.00000  -0.00105  -0.00105
4.94085
    R7        2.75082   0.00000   0.00000   0.00001   0.00001
2.75083
    R8        2.81856  -0.00002   0.00000   0.00000   0.00000
2.81856
```

This journal is © The Royal Society of Chemistry 2014

R9	2.73016	0.00000	0.00000	-0.00003	-0.00003
2.73014					
R10	5.19777	0.00000	0.00000	0.00008	0.00008
5.19786					
R11	2.66475	0.00000	0.00000	0.00000	0.00000
2.66475					
R12	2.05757	0.00000	0.00000	0.00000	0.00000
2.05757					
R13	3.87724	0.00000	0.00000	0.00031	0.00031
3.87755					
R14	4.51769	0.00000	0.00000	0.00026	0.00026
4.51794					
R15	2.73644	0.00000	0.00000	-0.00002	-0.00002
2.73642					
R16	4.69361	0.00001	0.00000	0.00040	0.00040
4.69401					
R17	2.04809	0.00000	0.00000	-0.00001	-0.00001
2.04809					
R18	2.67020	-0.00001	0.00000	-0.00001	-0.00001
2.67019					
R19	5.03584	0.00000	0.00000	-0.00002	-0.00002
5.03581					
R20	2.82401	0.00000	0.00000	-0.00004	-0.00004
2.82397					
R21	5.13332	0.00000	0.00000	-0.00013	-0.00013
5.13319					
R22	2.04293	0.00000	0.00000	-0.00001	-0.00001
2.04292					
R23	5.40426	0.00000	0.00000	-0.00067	-0.00067
5.40359					
R24	2.78465	0.00000	0.00000	0.00004	0.00004
2.78469					
R25	5.37413	0.00000	0.00000	-0.00074	-0.00074
5.37339					
R26	5.35738	0.00000	0.00000	-0.00094	-0.00094
5.35644					
R27	2.04963	0.00000	0.00000	0.00001	0.00001
2.04964					
R28	2.61810	0.00000	0.00000	0.00000	0.00000
2.61811					
R29	2.05319	0.00000	0.00000	0.00000	0.00000
2.05319					
R30	2.66280	0.00000	0.00000	0.00000	0.00000
2.66280					
R31	2.05282	0.00000	0.00000	0.00000	0.00000
2.05282					
R32	2.61671	0.00000	0.00000	0.00000	0.00000
2.61672					
R33	2.05361	0.00000	0.00000	0.00000	0.00000
2.05361					
R34	2.68951	0.00000	0.00000	0.00001	0.00001
2.68952					

This journal is © The Royal Society of Chemistry 2014

R35	2.66245	0.00000	0.00000	0.00001	0.00001
2.66246					
R36	2.67681	0.00001	0.00000	0.00001	0.00001
2.67682					
R37	2.04380	0.00000	0.00000	0.00000	0.00000
2.04380					
R38	2.62148	0.00000	0.00000	0.00000	0.00000
2.62149					
R39	4.19533	0.00002	0.00000	0.00018	0.00018
4.19551					
R40	2.05368	0.00000	0.00000	0.00000	0.00000
2.05368					
R41	2.66178	0.00000	0.00000	-0.00001	-0.00001
2.66177					
R42	2.05358	0.00000	0.00000	0.00000	0.00000
2.05358					
R43	2.61913	0.00000	0.00000	-0.00001	-0.00001
2.61912					
R44	2.05541	0.00000	0.00000	0.00000	0.00000
2.05541					
R45	2.65911	0.00000	0.00000	-0.00005	-0.00005
2.65906					
R46	2.27419	0.00000	0.00000	0.00000	0.00000
2.27419					
R47	2.62237	0.00000	0.00000	0.00003	0.00003
2.62239					
R48	2.27259	0.00000	0.00000	0.00000	0.00000
2.27258					
R49	2.08478	0.00001	0.00000	0.00002	0.00002
2.08480					
R50	2.30648	0.00000	0.00000	-0.00001	-0.00001
2.30646					
A1	2.04068	0.00000	0.00000	0.00001	0.00001
2.04070					
A2	2.17372	-0.00001	0.00000	-0.00004	-0.00004
2.17369					
A3	2.06849	0.00001	0.00000	0.00003	0.00003
2.06852					
A4	2.05285	0.00001	0.00000	0.00000	0.00000
2.05285					
A5	2.05939	-0.00002	0.00000	-0.00017	-0.00017
2.05922					
A6	2.13580	0.00001	0.00000	0.00012	0.00012
2.13591					
A7	2.03300	0.00000	0.00000	-0.00002	-0.00002
2.03299					
A8	2.10005	0.00000	0.00000	-0.00001	-0.00001
2.10003					
A9	2.14742	0.00001	0.00000	0.00004	0.00004
2.14745					
A10	2.03905	0.00000	0.00000	0.00003	0.00003
2.03908					

This journal is © The Royal Society of Chemistry 2014

A11	2.04254	0.00000	0.00000	0.00003	0.00003
2.04257					
A12	2.04691	0.00000	0.00000	0.00002	0.00002
2.04693					
A13	2.15543	0.00000	0.00000	0.00006	0.00006
2.15549					
A14	2.05497	0.00000	0.00000	0.00003	0.00003
2.05500					
A15	1.85395	0.00000	0.00000	0.00003	0.00003
1.85398					
A16	2.20979	0.00000	0.00000	-0.00002	-0.00002
2.20978					
A17	1.87908	0.00000	0.00000	-0.00003	-0.00003
1.87904					
A18	2.10091	0.00000	0.00000	-0.00005	-0.00005
2.10086					
A19	2.10383	0.00000	0.00000	-0.00002	-0.00002
2.10381					
A20	2.09941	0.00000	0.00000	-0.00002	-0.00002
2.09939					
A21	2.07932	0.00001	0.00000	0.00003	0.00003
2.07935					
A22	2.08532	0.00000	0.00000	0.00000	0.00000
2.08532					
A23	2.10835	0.00000	0.00000	-0.00001	-0.00001
2.10835					
A24	2.08952	0.00000	0.00000	0.00000	0.00000
2.08952					
A25	2.09276	0.00000	0.00000	-0.00001	-0.00001
2.09275					
A26	2.09468	0.00000	0.00000	0.00001	0.00001
2.09470					
A27	2.09574	0.00000	0.00000	0.00000	0.00000
2.09574					
A28	2.09461	0.00000	0.00000	-0.00001	-0.00001
2.09460					
A29	2.08278	0.00000	0.00000	0.00000	0.00000
2.08278					
A30	2.10571	0.00000	0.00000	0.00000	0.00000
2.10571					
A31	2.04124	0.00000	0.00000	0.00001	0.00001
2.04124					
A32	2.13703	0.00000	0.00000	-0.00002	-0.00002
2.13701					
A33	2.10082	0.00000	0.00000	0.00001	0.00001
2.10083					
A34	2.03013	0.00000	0.00000	-0.00003	-0.00003
2.03009					
A35	2.18261	0.00000	0.00000	0.00005	0.00005
2.18266					
A36	2.06939	0.00000	0.00000	-0.00002	-0.00002
2.06937					

A37	2.08506	-0.00001	0.00000	0.00002	0.00002	2.08507
A38	2.09606	0.00000	0.00000	0.00000	0.00000	2.09607
A39	2.10199	0.00001	0.00000	-0.00002	-0.00002	2.10197
A40	2.08294	0.00000	0.00000	-0.00001	-0.00001	2.08293
A41	2.11174	0.00000	0.00000	0.00001	0.00001	2.11175
A42	2.08850	0.00000	0.00000	0.00000	0.00000	2.08850
A43	2.09499	0.00000	0.00000	0.00000	0.00000	2.09499
A44	2.09199	0.00000	0.00000	-0.00001	-0.00001	2.09198
A45	2.09621	0.00000	0.00000	0.00000	0.00000	2.09621
A46	2.09545	0.00000	0.00000	0.00000	0.00000	2.09546
A47	2.08316	0.00000	0.00000	0.00000	0.00000	2.08316
A48	2.10432	0.00000	0.00000	0.00000	0.00000	2.10432
A49	1.88322	0.00000	0.00000	0.00001	0.00001	1.88323
A50	2.28817	0.00000	0.00000	-0.00002	-0.00002	2.28815
A51	2.11179	0.00000	0.00000	0.00001	0.00001	2.11180
A52	1.88817	0.00000	0.00000	-0.00001	-0.00001	1.88817
A53	2.26122	0.00000	0.00000	0.00002	0.00002	2.26124
A54	2.13357	0.00000	0.00000	-0.00002	-0.00002	2.13356
A55	1.90742	0.00000	0.00000	-0.00001	-0.00001	1.90742
A56	2.00161	-0.00001	0.00000	-0.00013	-0.00013	2.00148
A57	2.19148	0.00000	0.00000	0.00010	0.00010	2.19159
A58	2.08867	0.00001	0.00000	0.00004	0.00004	2.08871
D1	-0.56866	0.00000	0.00000	-0.00008	-0.00008	-0.56874
D2	2.84771	0.00000	0.00000	0.00009	0.00009	2.84779
D3	2.59915	0.00000	0.00000	-0.00015	-0.00015	2.59900
D4	-0.26767	0.00000	0.00000	0.00002	0.00002	-0.26765

This journal is © The Royal Society of Chemistry 2014

D5	-0.02869	0.00000	0.00000	0.00012	0.00012	-0.02857
D6	-3.09352	0.00000	0.00000	0.00005	0.00005	-3.09347
D7	3.08832	0.00000	0.00000	0.00019	0.00019	3.08851
D8	0.02350	0.00000	0.00000	0.00011	0.00011	0.02361
D9	-0.05532	0.00000	0.00000	-0.00006	-0.00006	-0.05538
D10	3.12470	0.00000	0.00000	-0.00004	-0.00004	3.12466
D11	3.11288	0.00000	0.00000	-0.00013	-0.00013	3.11275
D12	0.00971	0.00000	0.00000	-0.00011	-0.00011	0.00961
D13	0.56096	0.00000	0.00000	-0.00002	-0.00002	0.56094
D14	-2.63097	0.00000	0.00000	-0.00011	-0.00011	-2.63108
D15	-2.86825	-0.00001	0.00000	-0.00025	-0.00025	-2.86850
D16	0.22301	-0.00001	0.00000	-0.00034	-0.00034	0.22268
D17	-0.37674	0.00000	0.00000	-0.00132	-0.00132	-0.37806
D18	2.82267	-0.00002	0.00000	-0.00149	-0.00149	2.82118
D19	3.05349	0.00000	0.00000	-0.00112	-0.00112	3.05237
D20	-0.03029	-0.00002	0.00000	-0.00128	-0.00128	-0.03157
D21	-3.09387	0.00000	0.00000	0.00007	0.00007	-3.09380
D22	0.63108	0.00000	0.00000	-0.00007	-0.00007	0.63100
D23	-0.03133	0.00000	0.00000	0.00015	0.00015	-0.03118
D24	-2.58957	0.00000	0.00000	0.00000	0.00000	-2.58957
D25	-0.04154	0.00000	0.00000	-0.00004	-0.00004	-0.04158
D26	3.11394	0.00000	0.00000	-0.00002	-0.00002	3.11392
D27	-3.10116	0.00000	0.00000	-0.00012	-0.00012	-3.10128
D28	0.05433	0.00000	0.00000	-0.00010	-0.00010	0.05423
D29	-0.63845	0.00000	0.00000	-0.00003	-0.00003	-0.63848
D30	2.60011	0.00000	0.00000	0.00001	0.00001	2.60012

This journal is © The Royal Society of Chemistry 2014

D31	3.08915	0.00000	0.00000	-0.00018	-0.00018	3.08897
D32	0.04452	0.00000	0.00000	-0.00014	-0.00014	0.04438
D33	-0.16983	0.00000	0.00000	0.00022	0.00022	-0.16962
D34	2.51542	0.00000	0.00000	-0.00002	-0.00002	2.51540
D35	-2.62561	-0.00001	0.00000	0.00005	0.00005	-2.62556
D36	0.05964	0.00000	0.00000	-0.00018	-0.00018	0.05946
D37	-2.63576	0.00000	0.00000	-0.00006	-0.00006	-2.63582
D38	0.52849	0.00000	0.00000	-0.00005	-0.00005	0.52844
D39	-0.13356	0.00000	0.00000	0.00011	0.00011	-0.13345
D40	3.03069	0.00000	0.00000	0.00012	0.00012	3.03081
D41	0.03224	0.00000	0.00000	0.00020	0.00020	0.03244
D42	-3.10734	0.00000	0.00000	0.00020	0.00020	-3.10713
D43	2.75139	0.00001	0.00000	-0.00001	-0.00001	2.75138
D44	-0.38818	0.00000	0.00000	-0.00001	-0.00001	-0.38819
D45	3.11580	0.00000	0.00000	0.00002	0.00002	3.11582
D46	-0.02535	0.00000	0.00000	0.00003	0.00003	-0.02531
D47	0.01210	0.00000	0.00000	0.00004	0.00004	0.01214
D48	-3.12905	0.00000	0.00000	0.00006	0.00006	-3.12899
D49	-3.13267	0.00000	0.00000	0.00001	0.00001	-3.13266
D50	0.00739	0.00000	0.00000	0.00004	0.00004	0.00742
D51	0.00937	0.00000	0.00000	0.00002	0.00002	0.00939
D52	-3.13376	0.00000	0.00000	0.00005	0.00005	-3.13371
D53	0.02607	0.00000	0.00000	-0.00003	-0.00003	0.02604
D54	-3.12960	0.00000	0.00000	-0.00005	-0.00005	-3.12966
D55	-3.11706	0.00000	0.00000	0.00000	0.00000	-3.11706
D56	0.01045	0.00000	0.00000	-0.00002	-0.00002	0.01043

This journal is © The Royal Society of Chemistry 2014

D57	0.03932	0.00000	0.00000	0.00006	0.00006	0.03938
D58	-3.05536	0.00000	0.00000	0.00014	0.00014	-3.05522
D59	3.08607	0.00000	0.00000	0.00002	0.00002	3.08609
D60	-0.00861	0.00000	0.00000	0.00010	0.00010	-0.00851
D61	3.07880	0.00000	0.00000	-0.00009	-0.00009	3.07870
D62	-0.08671	0.00000	0.00000	-0.00006	-0.00006	-0.08678
D63	0.03739	0.00000	0.00000	-0.00005	-0.00005	0.03734
D64	-3.12812	0.00000	0.00000	-0.00002	-0.00002	-3.12814
D65	0.03831	-0.00001	0.00000	0.00002	0.00002	0.03832
D66	-3.11646	0.00000	0.00000	0.00002	0.00002	-3.11644
D67	3.12853	-0.00001	0.00000	-0.00007	-0.00007	3.12845
D68	-0.02624	0.00000	0.00000	-0.00007	-0.00007	-0.02631
D69	-3.10942	0.00000	0.00000	0.00000	0.00000	-3.10942
D70	0.03300	0.00000	0.00000	-0.00001	-0.00001	0.03299
D71	0.01887	0.00000	0.00000	0.00001	0.00001	0.01887
D72	-3.12189	0.00000	0.00000	-0.00001	-0.00001	-3.12190
D73	3.13914	0.00000	0.00000	0.00003	0.00003	3.13917
D74	-0.00405	0.00000	0.00000	0.00006	0.00006	-0.00399
D75	-0.00161	0.00000	0.00000	0.00002	0.00002	-0.00160
D76	3.13838	0.00000	0.00000	0.00005	0.00005	3.13843
D77	-0.03113	0.00000	0.00000	-0.00003	-0.00003	-0.03117
D78	3.13467	0.00000	0.00000	-0.00006	-0.00006	3.13461
D79	3.10886	0.00000	0.00000	0.00000	0.00000	3.10886
D80	-0.00853	0.00000	0.00000	-0.00003	-0.00003	-0.00856
D81	-0.11917	0.00000	0.00000	-0.00013	-0.00013	-0.11931
D82	3.02065	0.00000	0.00000	-0.00013	-0.00013	3.02051

```
   D83        0.15651   0.00000   0.00000   0.00002   0.00002
0.15653
   D84       -3.00573   0.00000   0.00000   0.00001   0.00001  -
3.00573
         Item               Value     Threshold  Converged?
 Maximum Force            0.000018     0.000450     YES
 RMS     Force            0.000004     0.000300     YES
 Maximum Displacement     0.002598     0.001800     NO
 RMS     Displacement     0.000327     0.001200     YES
 Predicted change in Energy=-4.205885D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.556107    0.522804    1.163074
    2          6             0        0.604218    1.084871    0.491060
    3          6             0       -0.741575   -0.883937    1.059937
    4          6             0        0.225762   -1.604694    0.264951
    5          1             0        0.063399   -2.674554    0.144253
    6          6             0       -0.203325   -0.963254   -1.636306
    7          1             0        0.492731   -1.645335   -2.110541
    8          6             0       -0.096097    0.443219   -1.719468
    9          1             0        0.737558    1.003762   -2.118865
   10          6             0       -1.515991    1.280964    1.877735
   11          1             0       -1.392996    2.351686    1.999537
   12          6             0       -2.601313    0.655007    2.469095
   13          1             0       -3.316615    1.245924    3.034467
   14          6             0       -2.786870   -0.736390    2.346086
   15          1             0       -3.647545   -1.211000    2.808730
   16          6             0       -1.873991   -1.496779    1.634839
   17          1             0       -2.012947   -2.568883    1.524144
   18          6             0        1.597331   -1.143561    0.319836
   19          6             0        1.802258    0.261873    0.411225
   20          6             0        3.128123    0.757807    0.359858
   21          1             0        3.299805    1.824167    0.415685
   22          6             0        4.196059   -0.121312    0.254637
   23          1             0        5.209662    0.270595    0.246566
   24          6             0        3.985055   -1.510569    0.157436
   25          1             0        4.833038   -2.184953    0.073389
   26          6             0        2.694260   -2.015150    0.171118
   27          1             0        2.517808   -3.085368    0.090234
   28          6             0       -1.461931    0.992773   -1.782442
   29          6             0       -1.661029   -1.277399   -1.734220
   30          8             0       -2.365284   -0.082378   -1.693131
   31          8             0       -2.211113   -2.343961   -1.812303
   32          8             0       -1.854896    2.125055   -1.891079
   33          6             0        0.628646    2.556572    0.249966
```

34	1	0	-0.362628	3.040774	0.255831
35	8	0	1.623006	3.218556	-0.000463

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.453917	0.000000			
3	C	1.422658	2.451731	0.000000		
4	C	2.438072	2.725457	1.444727	0.000000	
5	H	3.412460	3.813926	2.166280	1.088820	0.000000
6	C	3.188942	3.061474	2.750587	2.051911	2.483964
7	H	4.064166	3.772900	3.486426	2.390792	2.515495
8	C	2.920102	2.405949	3.146916	2.869749	3.635849
9	H	3.560339	2.614587	3.981962	3.570513	4.371064
10	C	1.416659	2.540985	2.440350	3.736549	4.598429
11	H	2.178270	2.805208	3.431684	4.613254	5.552139
12	C	2.430233	3.791151	2.795120	4.237552	4.857113
13	H	3.412538	4.676301	3.881482	5.323972	5.928572
14	C	2.821594	4.272890	2.420574	3.763114	4.090059
15	H	3.907844	5.359114	3.407331	4.650625	4.797138
16	C	2.457254	3.756949	1.410125	2.509422	2.713389
17	H	3.436755	4.611587	2.161231	2.743546	2.495291
18	C	2.850460	2.445710	2.466909	1.448054	2.174331
19	C	2.489026	1.455679	2.864402	2.447613	3.423084
20	C	3.778086	2.548388	4.261455	3.743544	4.606530
21	H	4.137655	2.796145	4.907305	4.607553	5.548557
22	C	4.880904	3.796327	5.060666	4.238372	4.859024
23	H	5.843603	4.683262	6.116514	5.325065	5.930295
24	C	5.076225	4.275239	4.852650	3.762008	4.090772
25	H	6.128804	5.361820	5.808806	4.647622	4.795226
26	C	4.241471	3.752435	3.724863	2.504149	2.712373
27	H	4.859922	4.605798	4.050951	2.734300	2.489138
28	C	3.117283	3.073478	3.481389	3.713080	4.414529
29	C	3.585513	3.957718	2.967747	2.768355	2.907637
30	O	3.434716	3.866665	3.295195	3.586789	3.999232
31	O	4.450872	4.998846	3.541324	3.286314	3.018412
32	O	3.685364	3.578241	4.359129	4.784206	5.555058
33	C	2.524603	1.491519	3.790866	4.180751	5.262638
34	H	2.683411	2.194466	4.024120	4.682591	5.732270
35	O	3.656423	2.414982	4.852437	5.028567	6.097710

		6	7	8	9	10
6	C	0.000000				
7	H	1.083802	0.000000			
8	C	1.413004	2.204929	0.000000		
9	H	2.233222	2.660399	1.081068	0.000000	
10	C	4.371280	5.338963	3.956992	4.596535	0.000000
11	H	5.061966	6.035303	4.376665	4.828809	1.084624
12	C	5.022293	5.986463	4.885184	5.684985	1.385443
13	H	6.032343	7.024357	5.797928	6.561386	2.140445
14	C	4.752433	5.607449	5.016021	5.948572	2.429857
15	H	5.628709	6.444358	5.987804	6.958124	3.408835
16	C	3.711625	4.432980	4.263317	5.211831	2.811231

This journal is © The Royal Society of Chemistry 2014

17	H	3.980103	4.510244	4.823701	5.796602	3.897861
18	C	2.664838	2.716367	3.089389	3.361171	4.242422
19	C	3.116999	3.422222	2.859456	2.843473	3.768286
20	C	4.247972	4.338577	3.849435	3.452442	4.913801
21	H	4.924662	5.128247	4.242410	3.696229	5.062069
22	C	4.862007	4.650952	4.757982	4.342872	6.101503
23	H	5.862424	5.610363	5.660933	5.111997	6.993995
24	C	4.589073	4.166318	4.898556	4.695705	6.404185
25	H	5.457156	4.888661	5.866685	5.634433	7.455093
26	C	3.573411	3.192094	4.171808	4.264568	5.612764
27	H	3.858609	3.319343	4.749572	4.976986	6.207378
28	C	2.330555	3.299692	1.473594	2.225097	3.671903
29	C	1.494381	2.217132	2.325888	3.332397	4.428598
30	O	2.335217	3.284100	2.329411	3.314902	3.915493
31	O	2.443059	2.808522	3.500041	4.471677	5.219163
32	O	3.511445	4.446948	2.439549	2.833725	3.877022
33	C	4.079139	4.821461	2.978285	2.834508	2.979308
34	H	4.431456	5.318925	3.274162	3.316474	2.656642
35	O	4.847577	5.421013	3.689552	3.190134	4.139467

		11	12	13	14	15
11	H	0.000000				
12	C	2.135235	0.000000			
13	H	2.448285	1.086501	0.000000		
14	C	3.405759	1.409095	2.164270	0.000000	
15	H	4.293077	2.166088	2.489366	1.086303	0.000000
16	C	3.895515	2.419744	3.400373	1.384707	2.145969
17	H	4.982202	3.410656	4.305041	2.152343	2.483127
18	C	4.896959	5.048046	6.101289	4.846927	5.805848
19	C	4.135179	4.876558	5.835462	5.079401	6.133330
20	C	5.066510	6.106216	6.994744	6.415986	7.468792
21	H	4.980888	6.356619	7.139285	6.879717	7.950130
22	C	6.355937	7.191019	8.126319	7.315312	8.320633
23	H	7.141355	8.130113	9.023362	8.328658	9.338626
24	C	6.872684	7.308469	8.318049	7.158807	8.085523
25	H	7.940695	8.311098	9.325006	8.082480	8.963870
26	C	6.254441	6.360308	7.413770	6.033946	6.915355
27	H	6.964293	6.771616	7.840222	6.224643	6.993929
28	C	4.019299	4.414503	5.167838	4.667999	5.541875
29	C	5.213736	4.720825	5.643448	4.267214	4.958735
30	O	4.528334	4.233624	5.001959	4.113483	4.815053
31	O	6.103159	5.241797	6.131932	4.495329	4.969999
32	O	3.924488	4.661469	5.212532	5.197115	6.035814
33	C	2.681421	4.355814	5.003632	5.186817	6.247214
34	H	2.139396	3.949953	4.434901	4.951069	5.948575
35	O	3.721254	5.524071	6.123882	6.371413	7.435808

		16	17	18	19	20
16	C	0.000000				
17	H	1.086725	0.000000			
18	C	3.728817	4.063989	0.000000		
19	C	4.254985	4.879299	1.423232	0.000000	
20	C	5.632928	6.233220	2.441337	1.416512	0.000000
21	H	6.267629	6.982327	3.422720	2.164123	1.081533

This journal is © The Royal Society of Chemistry 2014

22	C	6.375138	6.793674	2.793319	2.429328	1.387231
23	H	7.431626	7.865172	3.879967	3.411391	2.140798
24	C	6.042460	6.242110	2.421217	2.823218	2.433277
25	H	6.920690	7.008538	3.408083	3.909823	3.413009
26	C	4.824946	4.929005	1.408913	2.457265	2.813032
27	H	4.919077	4.780229	2.161159	3.437887	3.900663
28	C	4.247996	4.891066	4.282824	4.000165	5.070824
29	C	3.382904	3.522601	3.854085	4.355072	5.609207
30	O	3.649286	4.081386	4.569515	4.681371	5.924373
31	O	3.565692	3.349887	4.526724	5.276514	6.545738
32	O	5.054715	5.807046	5.243078	4.706041	5.636183
33	C	4.960919	5.905238	3.825470	2.582444	3.081399
34	H	4.977476	5.983346	4.621060	3.526070	4.172302
35	O	6.094061	7.002788	4.373936	2.990585	2.906974

		21	22	23	24	25
21	H	0.000000				
22	C	2.148045	0.000000			
23	H	2.467740	1.086760	0.000000		
24	C	3.414194	1.408548	2.163367	0.000000	
25	H	4.305927	2.167304	2.490291	1.086707	0.000000
26	C	3.894464	2.418470	3.399643	1.385980	2.147733
27	H	4.982064	3.410159	4.304998	2.153444	2.484215
28	C	5.310095	6.115860	7.010604	6.300755	7.291686
29	C	6.233111	6.292660	7.316160	5.959110	6.801765
30	O	6.338395	6.844454	7.827313	6.766915	7.704366
31	O	7.259989	7.089730	8.132820	6.554915	7.293914
32	O	5.655319	6.801788	7.610291	7.177688	8.195350
33	C	2.774702	4.460664	5.119708	5.274058	6.339570
34	H	3.862525	5.548010	6.222893	6.294978	7.371326
35	O	2.220171	4.223790	4.649258	5.288557	6.285513

		26	27	28	29	30
26	C	0.000000				
27	H	1.087678	0.000000			
28	C	5.489802	5.998039	0.000000		
29	C	4.810731	4.905105	2.279396	0.000000	
30	O	5.728003	6.003576	1.407115	1.387710	0.000000
31	O	5.301393	5.150924	3.419936	1.202599	2.269963
32	O	6.487586	7.084817	1.203447	3.411581	2.274299
33	C	5.017332	5.951969	3.308574	4.886608	4.438840
34	H	5.908816	6.771554	3.091493	4.928769	4.190842
35	O	5.344970	6.367759	4.200761	5.831330	5.446811

		31	32	33	34	35
31	O	0.000000				
32	O	4.483882	0.000000			
33	C	6.027637	3.307304	0.000000		
34	H	6.057181	2.770312	1.103227	0.000000	
35	O	6.994629	4.106820	1.220528	2.009984	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1

This journal is © The Royal Society of Chemistry 2014

```
 Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.521135    0.690568    1.079231
    2          6             0        0.627166    1.131740    0.304218
    3          6             0       -0.724131   -0.713345    1.187756
    4          6             0        0.214454   -1.556303    0.483687
    5          1             0        0.037668   -2.629882    0.524947
    6          6             0       -0.257234   -1.193528   -1.480045
    7          1             0        0.418951   -1.947474   -1.866005
    8          6             0       -0.137307    0.184013   -1.770869
    9          1             0        0.691546    0.668191   -2.268143
   10          6             0       -1.453969    1.558677    1.698207
   11          1             0       -1.316497    2.633834    1.658866
   12          6             0       -2.530077    1.041448    2.400998
   13          1             0       -3.224092    1.718812    2.890903
   14          6             0       -2.733518   -0.350190    2.487627
   15          1             0       -3.586820   -0.739736    3.035517
   16          6             0       -1.847606   -1.219333    1.873493
   17          1             0       -2.000757   -2.294007    1.924407
   18          6             0        1.591800   -1.111763    0.437180
   19          6             0        1.813927    0.288862    0.316757
   20          6             0        3.143184    0.752952    0.161186
   21          1             0        3.327557    1.813456    0.056061
   22          6             0        4.198635   -0.147288    0.159995
   23          1             0        5.215780    0.224696    0.070045
   24          6             0        3.970453   -1.532674    0.272448
   25          1             0        4.808760   -2.224157    0.267542
   26          6             0        2.675177   -2.011325    0.391167
   27          1             0        2.485341   -3.079240    0.472194
   28          6             0       -1.498417    0.737941   -1.880521
   29          6             0       -1.720243   -1.497729   -1.495530
   30          8             0       -2.410481   -0.299585   -1.612841
   31          8             0       -2.283452   -2.556274   -1.403211
   32          8             0       -1.882056    1.847693   -2.144255
   33          6             0        0.660899    2.551906   -0.150335
   34          1             0       -0.324696    3.045893   -0.191418
   35          8             0        1.655353    3.155897   -0.519043
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3890030      0.2596864
0.2420830
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
```

Supplementary Material (ESI) for Green Chemistry
This journal is © The Royal Society of Chemistry 2014

```
      nuclear repulsion energy      1906.9628679474 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
```

This journal is © The Royal Society of Chemistry 2014

```
 SCF Done:  E(RB+HF-LYP) =  -1032.13801903     A.U. after   13 cycles
            Convg  =    0.5983D-08             -V/T =  2.0093
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000003800   -0.000000596   -0.000004659
    2          6          -0.000002623   -0.000000037    0.000006427
    3          6           0.000000482   -0.000000966   -0.000000391
    4          6           0.000002628    0.000001956   -0.000003825
    5          1           0.000001772    0.000000480   -0.000001462
    6          6           0.000003515   -0.000001038    0.000003553
    7          1           0.000000142    0.000001266   -0.000002060
    8          6          -0.000004038   -0.000000168   -0.000003374
    9          1           0.000001348    0.000003927    0.000005409
   10          6           0.000000645   -0.000001761    0.000001296
   11          1           0.000000812   -0.000000576    0.000001776
   12          6          -0.000000873   -0.000003219    0.000000249
   13          1          -0.000001047   -0.000003957    0.000000610
   14          6           0.000000468   -0.000002933   -0.000000200
   15          1           0.000000666   -0.000004006   -0.000000740
   16          6           0.000001606   -0.000002124   -0.000000854
   17          1           0.000001617   -0.000002220   -0.000001461
   18          6           0.000000555   -0.000002027    0.000000311
   19          6          -0.000003198   -0.000000006   -0.000001927
   20          6           0.000005751    0.000001274    0.000003888
   21          1           0.000000640   -0.000000753   -0.000001671
   22          6          -0.000000287    0.000002997    0.000000260
   23          1          -0.000000180    0.000003136    0.000000633
   24          6          -0.000000675    0.000003135   -0.000000591
   25          1           0.000001398    0.000003312   -0.000000973
   26          6           0.000002783    0.000002085   -0.000000819
   27          1           0.000002323    0.000001638   -0.000001480
   28          6           0.000000779    0.000000667    0.000000910
   29          6          -0.000000341    0.000000143   -0.000000621
   30          8          -0.000000137   -0.000001589    0.000000622
   31          8           0.000001644   -0.000001067   -0.000001105
   32          8          -0.000001984    0.000000075    0.000000083
   33          6          -0.000000091   -0.000000825   -0.000006538
   34          1          -0.000004583   -0.000000591    0.000002019
   35          8          -0.000007719    0.000004370    0.000006705
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000007719 RMS     0.000002488


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000005895 RMS     0.000001299
 Search for a saddle point.
```

This journal is © The Royal Society of Chemistry 2014

```
 Step number  11 out of a maximum of 202
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Update second derivatives using D2CorX and points  4  5  6  7  8
                                                     9 10 11
     Eigenvalues ---   -0.01896   0.00238   0.00433   0.00708
0.00853
     Eigenvalues ---    0.01010   0.01264   0.01442   0.01484
0.01540
     Eigenvalues ---    0.01642   0.01672   0.01775   0.01880
0.01929
     Eigenvalues ---    0.01989   0.02132   0.02174   0.02188
0.02234
     Eigenvalues ---    0.02363   0.02427   0.02449   0.02520
0.02657
     Eigenvalues ---    0.02715   0.02746   0.02748   0.03019
0.03504
     Eigenvalues ---    0.03988   0.05546   0.07030   0.07372
0.07482
     Eigenvalues ---    0.08785   0.10170   0.11043   0.11179
0.11222
     Eigenvalues ---    0.11861   0.12276   0.12499   0.12527
0.12659
     Eigenvalues ---    0.12832   0.13903   0.14245   0.14648
0.16399
     Eigenvalues ---    0.17651   0.18497   0.19087   0.19169
0.19333
     Eigenvalues ---    0.19414   0.20108   0.20396   0.20897
0.21162
     Eigenvalues ---    0.23350   0.23904   0.24403   0.25102
0.26059
     Eigenvalues ---    0.27637   0.27925   0.29100   0.30147
0.30311
     Eigenvalues ---    0.31234   0.33068   0.33987   0.34004
0.34999
     Eigenvalues ---    0.35270   0.35918   0.36086   0.36133
0.36201
     Eigenvalues ---    0.36237   0.36329   0.36535   0.37390
0.37810
     Eigenvalues ---    0.38851   0.39854   0.40316   0.41108
0.42458
     Eigenvalues ---    0.44477   0.46223   0.47304   0.47636
0.50256
     Eigenvalues ---    0.50615   0.79374   0.89039
0.902551000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
         1             -0.04239   0.02322   0.14830   0.01769
0.35681
                           R6        R7        R8        R9        R10
         1              0.09488  -0.04288  -0.02011  -0.06200
0.19790
                           R11       R12       R13       R14       R15
         1              0.01925  -0.00714   0.45278   0.18950  -
0.05980
                           R16       R17       R18       R19       R20
         1              0.29981  -0.00770  -0.09458   0.18841  -
0.01425
                           R21       R22       R23       R24       R25
         1             -0.02912  -0.00686   0.15161  -0.00488  -
0.04078
                           R26       R27       R28       R29       R30
         1              0.06231  -0.00134  -0.01348   0.00008
0.01445
                           R31       R32       R33       R34       R35
```

This journal is © The Royal Society of Chemistry 2014

1	-0.00024	-0.01608	-0.00025	0.02111	0.01851

	R36	R37	R38	R39	R40
1	0.01774	-0.00152	-0.01221	-0.04587	0.00008

	R41	R42	R43	R44	R45
1	0.01317	-0.00013	-0.01559	-0.00013	0.00156

	R46	R47	R48	R49	R50
1	0.00076	-0.00098	0.00267	-0.00107	0.00482

	A1	A2	A3	A4	A5
1	0.02097	-0.00767	-0.01320	0.03161	-0.00431

	A6	A7	A8	A9	A10
1	0.00719	0.01906	-0.00138	-0.01646	0.03370

	A11	A12	A13	A14	A15
1	0.05743	0.03043	0.06346	0.04345	0.02333

	A16	A17	A18	A19	A20
1	0.04612	0.00663	0.01558	-0.00374	0.00676

	A21	A22	A23	A24	A25
1	-0.00311	-0.00136	0.00490	-0.00354	-0.00137

	A26	A27	A28	A29	A30
1	-0.00133	0.00271	0.00409	-0.00661	0.00244

	A31	A32	A33	A34	A35
1	0.01966	-0.01812	-0.00057	0.02078	-0.00712

	A36	A37	A38	A39	A40
1	-0.01365	-0.00324	0.00704	-0.00381	-0.00110

	A41	A42	A43	A44	A45
1	0.00450	-0.00340	-0.00109	-0.00155	0.00264

	A46	A47	A48	A49	A50
1	0.00422	-0.00637	0.00205	-0.00234	0.00159

	A51	A52	A53	A54	A55
1	0.00075	-0.00673	0.00460	0.00223	-0.01366

	A56	A57	A58	D1	D2
1	-0.00149	0.00949	-0.00807	0.13007	-0.00257

	D3	D4	D5	D6	D7
1	0.12536	-0.00728	0.02231	0.00587	0.02677

	D8	D9	D10	D11	D12

```
          1              0.01033  -0.00489  -0.00202  -0.01014  -
0.00727
                           D13       D14       D15       D16       D17
          1             -0.13426  -0.13445   0.00292   0.00273
0.08201
                           D18       D19       D20       D21       D22
          1              0.08346  -0.06127  -0.05982   0.05491  -
0.16108
                           D23       D24       D25       D26       D27
          1              0.07263  -0.14336  -0.00611   0.00053  -
0.02534
                           D28       D29       D30       D31       D32
          1             -0.01869   0.15669   0.14507  -0.06144  -
0.07307
                           D33       D34       D35       D36       D37
          1              0.02191   0.18031  -0.16715  -0.00876  -
0.15408
                           D38       D39       D40       D41       D42
          1             -0.15902   0.03195   0.02702  -0.01654  -
0.01462
                           D43       D44       D45       D46       D47
          1              0.13980   0.14172  -0.00133  -0.00041
0.00152
                           D48       D49       D50       D51       D52
          1              0.00244   0.00050   0.00491   0.00142
0.00583
                           D53       D54       D55       D56       D57
          1             -0.00158  -0.00839   0.00283  -0.00398  -
0.01337
                           D58       D59       D60       D61       D62
          1             -0.01331  -0.00307  -0.00300   0.01463
0.01021
                           D63       D64       D65       D66       D67
          1              0.00157  -0.00285   0.00225   0.00121
0.00296
                           D68       D69       D70       D71       D72
          1              0.00192   0.00217   0.00093   0.00112  -
0.00012
                           D73       D74       D75       D76       D77
          1              0.00087  -0.00227  -0.00038  -0.00352
0.00104
                           D78       D79       D80       D81       D82
          1              0.00563  -0.00211   0.00248   0.03904
0.03735
                           D83       D84
          1             -0.04639  -0.04185
 RFO step:  Lambda0=7.079616407D-11 Lambda=-1.32211008D-08.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.00018673 RMS(Int)=  0.00000008
 Iteration  2 RMS(Cart)=  0.00000011 RMS(Int)=  0.00000002
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
```

This journal is © The Royal Society of Chemistry 2014

			(Linear)	(Quad)	(Total)	
R1	2.74751	-0.00001	0.00000	-0.00003	-0.00003	2.74748
R2	2.68843	0.00000	0.00000	-0.00001	-0.00001	2.68842
R3	5.51819	0.00000	0.00000	0.00006	0.00006	5.51826
R4	2.67710	0.00000	0.00000	0.00000	0.00000	2.67710
R5	4.54658	0.00000	0.00000	0.00022	0.00022	4.54681
R6	4.94085	0.00000	0.00000	0.00005	0.00005	4.94090
R7	2.75083	0.00000	0.00000	-0.00001	-0.00001	2.75082
R8	2.81856	0.00000	0.00000	0.00001	0.00001	2.81857
R9	2.73014	0.00000	0.00000	0.00000	0.00000	2.73014
R10	5.19786	0.00000	0.00000	-0.00006	-0.00006	5.19780
R11	2.66475	0.00000	0.00000	0.00000	0.00000	2.66475
R12	2.05757	0.00000	0.00000	0.00000	0.00000	2.05757
R13	3.87755	0.00000	0.00000	-0.00009	-0.00009	3.87746
R14	4.51794	0.00000	0.00000	-0.00005	-0.00005	4.51789
R15	2.73642	0.00000	0.00000	0.00000	0.00000	2.73643
R16	4.69401	0.00000	0.00000	-0.00008	-0.00008	4.69393
R17	2.04809	0.00000	0.00000	0.00000	0.00000	2.04809
R18	2.67019	0.00000	0.00000	0.00000	0.00000	2.67019
R19	5.03581	0.00000	0.00000	-0.00005	-0.00005	5.03576
R20	2.82397	0.00000	0.00000	0.00002	0.00002	2.82399
R21	5.13319	0.00000	0.00000	0.00000	0.00000	5.13319
R22	2.04292	0.00000	0.00000	0.00000	0.00000	2.04292
R23	5.40359	0.00000	0.00000	0.00007	0.00007	5.40366
R24	2.78469	0.00000	0.00000	-0.00003	-0.00003	2.78466
R25	5.37339	0.00000	0.00000	-0.00010	-0.00010	5.37329

This journal is © The Royal Society of Chemistry 2014

R26	5.35644	0.00000	0.00000	0.00019	0.00019
5.35664					
R27	2.04964	0.00000	0.00000	0.00001	0.00001
2.04965					
R28	2.61811	0.00000	0.00000	0.00000	0.00000
2.61811					
R29	2.05319	0.00000	0.00000	0.00000	0.00000
2.05319					
R30	2.66280	0.00000	0.00000	0.00000	0.00000
2.66281					
R31	2.05282	0.00000	0.00000	0.00000	0.00000
2.05282					
R32	2.61672	0.00000	0.00000	0.00000	0.00000
2.61672					
R33	2.05361	0.00000	0.00000	0.00000	0.00000
2.05361					
R34	2.68952	0.00000	0.00000	0.00001	0.00001
2.68953					
R35	2.66246	0.00000	0.00000	0.00000	0.00000
2.66246					
R36	2.67682	0.00000	0.00000	0.00002	0.00002
2.67684					
R37	2.04380	0.00000	0.00000	0.00000	0.00000
2.04380					
R38	2.62149	0.00000	0.00000	-0.00001	-0.00001
2.62148					
R39	4.19551	0.00001	0.00000	0.00003	0.00003
4.19555					
R40	2.05368	0.00000	0.00000	0.00000	0.00000
2.05368					
R41	2.66177	0.00000	0.00000	0.00000	0.00000
2.66177					
R42	2.05358	0.00000	0.00000	0.00000	0.00000
2.05358					
R43	2.61912	0.00000	0.00000	0.00000	0.00000
2.61912					
R44	2.05541	0.00000	0.00000	0.00000	0.00000
2.05541					
R45	2.65906	0.00000	0.00000	0.00001	0.00001
2.65907					
R46	2.27419	0.00000	0.00000	0.00000	0.00000
2.27419					
R47	2.62239	0.00000	0.00000	-0.00001	-0.00001
2.62238					
R48	2.27258	0.00000	0.00000	0.00000	0.00000
2.27258					
R49	2.08480	0.00000	0.00000	0.00001	0.00001
2.08481					
R50	2.30646	0.00000	0.00000	-0.00001	-0.00001
2.30646					
A1	2.04070	0.00000	0.00000	0.00002	0.00002
2.04072					

This journal is © The Royal Society of Chemistry 2014

A2	2.17369	0.00000	0.00000	-0.00004	-0.00004
2.17364					
A3	2.06852	0.00000	0.00000	0.00002	0.00002
2.06854					
A4	2.05285	0.00000	0.00000	0.00003	0.00003
2.05288					
A5	2.05922	0.00000	0.00000	-0.00007	-0.00007
2.05915					
A6	2.13591	0.00000	0.00000	0.00006	0.00006
2.13598					
A7	2.03299	0.00000	0.00000	-0.00001	-0.00001
2.03298					
A8	2.10003	0.00000	0.00000	-0.00001	-0.00001
2.10002					
A9	2.14745	0.00000	0.00000	0.00002	0.00002
2.14747					
A10	2.03908	0.00000	0.00000	-0.00001	-0.00001
2.03907					
A11	2.04257	0.00000	0.00000	0.00000	0.00000
2.04258					
A12	2.04693	0.00000	0.00000	-0.00001	-0.00001
2.04692					
A13	2.15549	0.00000	0.00000	-0.00001	-0.00001
2.15548					
A14	2.05500	0.00000	0.00000	-0.00002	-0.00002
2.05498					
A15	1.85398	0.00000	0.00000	-0.00001	-0.00001
1.85397					
A16	2.20978	0.00000	0.00000	0.00002	0.00002
2.20980					
A17	1.87904	0.00000	0.00000	0.00001	0.00001
1.87906					
A18	2.10086	0.00000	0.00000	0.00001	0.00001
2.10087					
A19	2.10381	0.00000	0.00000	-0.00002	-0.00002
2.10379					
A20	2.09939	0.00000	0.00000	-0.00001	-0.00001
2.09938					
A21	2.07935	0.00000	0.00000	0.00003	0.00003
2.07938					
A22	2.08532	0.00000	0.00000	0.00001	0.00001
2.08533					
A23	2.10835	0.00000	0.00000	-0.00001	-0.00001
2.10834					
A24	2.08952	0.00000	0.00000	0.00000	0.00000
2.08952					
A25	2.09275	0.00000	0.00000	0.00000	0.00000
2.09274					
A26	2.09470	0.00000	0.00000	0.00001	0.00001
2.09471					
A27	2.09574	0.00000	0.00000	0.00000	0.00000
2.09574					

This journal is © The Royal Society of Chemistry 2014

A28	2.09460	0.00000	0.00000	0.00000	0.00000
2.09460					
A29	2.08278	0.00000	0.00000	0.00000	0.00000
2.08279					
A30	2.10571	0.00000	0.00000	0.00000	0.00000
2.10571					
A31	2.04124	0.00000	0.00000	0.00001	0.00001
2.04125					
A32	2.13701	0.00000	0.00000	-0.00001	-0.00001
2.13700					
A33	2.10083	0.00000	0.00000	0.00000	0.00000
2.10083					
A34	2.03009	0.00000	0.00000	0.00000	0.00000
2.03009					
A35	2.18266	0.00000	0.00000	0.00001	0.00001
2.18267					
A36	2.06937	0.00000	0.00000	-0.00001	-0.00001
2.06936					
A37	2.08507	0.00000	0.00000	0.00000	0.00000
2.08507					
A38	2.09607	0.00000	0.00000	0.00000	0.00000
2.09607					
A39	2.10197	0.00000	0.00000	0.00000	0.00000
2.10197					
A40	2.08293	0.00000	0.00000	0.00000	0.00000
2.08293					
A41	2.11175	0.00000	0.00000	0.00000	0.00000
2.11175					
A42	2.08850	0.00000	0.00000	0.00000	0.00000
2.08850					
A43	2.09499	0.00000	0.00000	0.00000	0.00000
2.09499					
A44	2.09198	0.00000	0.00000	0.00000	0.00000
2.09198					
A45	2.09621	0.00000	0.00000	0.00000	0.00000
2.09621					
A46	2.09546	0.00000	0.00000	0.00000	0.00000
2.09546					
A47	2.08316	0.00000	0.00000	0.00000	0.00000
2.08316					
A48	2.10432	0.00000	0.00000	0.00000	0.00000
2.10432					
A49	1.88323	0.00000	0.00000	0.00000	0.00000
1.88323					
A50	2.28815	0.00000	0.00000	0.00001	0.00001
2.28816					
A51	2.11180	0.00000	0.00000	-0.00001	-0.00001
2.11179					
A52	1.88817	0.00000	0.00000	0.00000	0.00000
1.88817					
A53	2.26124	0.00000	0.00000	-0.00001	-0.00001
2.26123					

This journal is © The Royal Society of Chemistry 2014

A54	2.13356	0.00000	0.00000	0.00001	0.00001	2.13356
A55	1.90742	0.00000	0.00000	0.00000	0.00000	1.90742
A56	2.00148	0.00000	0.00000	-0.00006	-0.00006	2.00142
A57	2.19159	0.00000	0.00000	0.00005	0.00005	2.19164
A58	2.08871	0.00000	0.00000	0.00002	0.00002	2.08872
D1	-0.56874	0.00000	0.00000	0.00009	0.00009	-0.56865
D2	2.84779	0.00000	0.00000	0.00000	0.00000	2.84779
D3	2.59900	0.00000	0.00000	-0.00001	-0.00001	2.59899
D4	-0.26765	0.00000	0.00000	-0.00010	-0.00010	-0.26775
D5	-0.02857	0.00000	0.00000	-0.00005	-0.00005	-0.02862
D6	-3.09347	0.00000	0.00000	-0.00006	-0.00006	-3.09353
D7	3.08851	0.00000	0.00000	0.00004	0.00004	3.08855
D8	0.02361	0.00000	0.00000	0.00004	0.00004	0.02364
D9	-0.05538	0.00000	0.00000	0.00003	0.00003	-0.05535
D10	3.12466	0.00000	0.00000	0.00006	0.00006	3.12472
D11	3.11275	0.00000	0.00000	-0.00007	-0.00007	3.11268
D12	0.00961	0.00000	0.00000	-0.00004	-0.00004	0.00957
D13	0.56094	0.00000	0.00000	-0.00009	-0.00009	0.56084
D14	-2.63108	0.00000	0.00000	-0.00012	-0.00012	-2.63120
D15	-2.86850	0.00000	0.00000	-0.00002	-0.00002	-2.86851
D16	0.22268	0.00000	0.00000	-0.00005	-0.00005	0.22263
D17	-0.37806	0.00000	0.00000	-0.00076	-0.00076	-0.37882
D18	2.82118	-0.00001	0.00000	-0.00086	-0.00086	2.82033
D19	3.05237	0.00000	0.00000	-0.00085	-0.00085	3.05152
D20	-0.03157	-0.00001	0.00000	-0.00095	-0.00095	-0.03252
D21	-3.09380	0.00000	0.00000	-0.00003	-0.00003	-3.09382

This journal is © The Royal Society of Chemistry 2014

D22	0.63100	0.00000	0.00000	0.00000	0.00000	0.63100
D23	-0.03118	0.00000	0.00000	-0.00002	-0.00002	-0.03120
D24	-2.58957	0.00000	0.00000	0.00000	0.00000	-2.58956
D25	-0.04158	0.00000	0.00000	-0.00001	-0.00001	-0.04159
D26	3.11392	0.00000	0.00000	-0.00001	-0.00001	3.11392
D27	-3.10128	0.00000	0.00000	-0.00002	-0.00002	-3.10130
D28	0.05423	0.00000	0.00000	-0.00001	-0.00001	0.05422
D29	-0.63848	0.00000	0.00000	0.00000	0.00000	-0.63848
D30	2.60012	0.00000	0.00000	0.00004	0.00004	2.60016
D31	3.08897	0.00000	0.00000	0.00003	0.00003	3.08900
D32	0.04438	0.00000	0.00000	0.00006	0.00006	0.04445
D33	-0.16962	0.00000	0.00000	-0.00018	-0.00018	-0.16980
D34	2.51540	0.00000	0.00000	-0.00006	-0.00006	2.51534
D35	-2.62556	0.00000	0.00000	-0.00012	-0.00012	-2.62568
D36	0.05946	0.00000	0.00000	-0.00001	-0.00001	0.05946
D37	-2.63582	0.00000	0.00000	0.00005	0.00005	-2.63577
D38	0.52844	0.00000	0.00000	0.00005	0.00005	0.52849
D39	-0.13345	0.00000	0.00000	0.00000	0.00000	-0.13345
D40	3.03081	0.00000	0.00000	0.00000	0.00000	3.03081
D41	0.03244	0.00000	0.00000	0.00001	0.00001	0.03245
D42	-3.10713	0.00000	0.00000	0.00003	0.00003	-3.10711
D43	2.75138	0.00000	0.00000	0.00012	0.00012	2.75151
D44	-0.38819	0.00000	0.00000	0.00014	0.00014	-0.38805
D45	3.11582	0.00000	0.00000	0.00000	0.00000	3.11582
D46	-0.02531	0.00000	0.00000	0.00002	0.00002	-0.02529
D47	0.01214	0.00000	0.00000	0.00003	0.00003	0.01217

This journal is © The Royal Society of Chemistry 2014

D48	-3.12899	0.00000	0.00000	0.00005	0.00005	-3.12894
D49	-3.13266	0.00000	0.00000	-0.00001	-0.00001	-3.13267
D50	0.00742	0.00000	0.00000	0.00001	0.00001	0.00743
D51	0.00939	0.00000	0.00000	0.00001	0.00001	0.00940
D52	-3.13371	0.00000	0.00000	0.00002	0.00002	-3.13368
D53	0.02604	0.00000	0.00000	-0.00001	-0.00001	0.02603
D54	-3.12966	0.00000	0.00000	-0.00001	-0.00002	-3.12967
D55	-3.11706	0.00000	0.00000	0.00000	0.00000	-3.11706
D56	0.01043	0.00000	0.00000	0.00000	0.00000	0.01042
D57	0.03938	0.00000	0.00000	0.00005	0.00005	0.03943
D58	-3.05522	0.00000	0.00000	0.00007	0.00007	-3.05515
D59	3.08609	0.00000	0.00000	0.00001	0.00001	3.08610
D60	-0.00851	0.00000	0.00000	0.00004	0.00004	-0.00847
D61	3.07870	0.00000	0.00000	-0.00005	-0.00005	3.07865
D62	-0.08678	0.00000	0.00000	-0.00004	-0.00004	-0.08681
D63	0.03734	0.00000	0.00000	-0.00002	-0.00002	0.03733
D64	-3.12814	0.00000	0.00000	0.00000	0.00000	-3.12814
D65	0.03832	0.00000	0.00000	0.00000	0.00000	0.03832
D66	-3.11644	0.00000	0.00000	0.00000	0.00000	-3.11644
D67	3.12845	0.00000	0.00000	-0.00003	-0.00003	3.12842
D68	-0.02631	0.00000	0.00000	-0.00003	-0.00003	-0.02633
D69	-3.10942	0.00000	0.00000	0.00000	0.00000	-3.10942
D70	0.03299	0.00000	0.00000	-0.00001	-0.00001	0.03299
D71	0.01887	0.00000	0.00000	0.00000	0.00000	0.01888
D72	-3.12190	0.00000	0.00000	0.00000	0.00000	-3.12190
D73	3.13917	0.00000	0.00000	0.00001	0.00001	3.13918

```
   D74       -0.00399   0.00000   0.00000   0.00003   0.00003  -
0.00396
   D75       -0.00160   0.00000   0.00000   0.00001   0.00001  -
0.00159
   D76        3.13843   0.00000   0.00000   0.00002   0.00002
3.13845
   D77       -0.03117   0.00000   0.00000  -0.00002  -0.00002  -
0.03118
   D78        3.13461   0.00000   0.00000  -0.00003  -0.00003
3.13458
   D79        3.10886   0.00000   0.00000   0.00000   0.00000
3.10885
   D80       -0.00856   0.00000   0.00000  -0.00001  -0.00001  -
0.00857
   D81       -0.11931   0.00000   0.00000  -0.00002  -0.00002  -
0.11932
   D82        3.02051   0.00000   0.00000  -0.00003  -0.00003
3.02049
   D83        0.15653   0.00000   0.00000   0.00001   0.00001
0.15654
   D84       -3.00573   0.00000   0.00000   0.00001   0.00001  -
3.00572
         Item               Value     Threshold  Converged?
 Maximum Force            0.000006     0.000450     YES
 RMS     Force            0.000001     0.000300     YES
 Maximum Displacement     0.001949     0.001800     NO
 RMS     Displacement     0.000187     0.001200     YES
 Predicted change in Energy=-6.575444D-09

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.556113    0.522802    1.163068
    2          6             0        0.604236    1.084877    0.491137
    3          6             0       -0.741590   -0.883932    1.059931
    4          6             0        0.225759   -1.604686    0.264955
    5          1             0        0.063405   -2.674549    0.144277
    6          6             0       -0.203307   -0.963299   -1.636273
    7          1             0        0.492734   -1.645395   -2.110509
    8          6             0       -0.096082    0.443172   -1.719503
    9          1             0        0.737608    1.003723   -2.118812
   10          6             0       -1.515956    1.280988    1.877755
   11          1             0       -1.392886    2.351701    1.999589
   12          6             0       -2.601292    0.655053    2.469110
   13          1             0       -3.316575    1.245974    3.034503
   14          6             0       -2.786878   -0.736341    2.346083
   15          1             0       -3.647561   -1.210936    2.808727
```

16	6	0	-1.874016	-1.496751	1.634832
17	1	0	-2.012995	-2.568853	1.524141
18	6	0	1.597330	-1.143555	0.319853
19	6	0	1.802266	0.261882	0.411251
20	6	0	3.128142	0.757808	0.359806
21	1	0	3.299835	1.824166	0.415609
22	6	0	4.196064	-0.121318	0.254537
23	1	0	5.209670	0.270581	0.246405
24	6	0	3.985047	-1.510576	0.157369
25	1	0	4.833022	-2.184965	0.073295
26	6	0	2.694251	-2.015147	0.171099
27	1	0	2.517791	-3.085364	0.090212
28	6	0	-1.461898	0.992730	-1.782536
29	6	0	-1.661021	-1.277436	-1.734200
30	8	0	-2.365266	-0.082413	-1.693177
31	8	0	-2.211104	-2.344001	-1.812240
32	8	0	-1.854859	2.125007	-1.891262
33	6	0	0.628568	2.556595	0.250093
34	1	0	-0.362838	3.040545	0.255181
35	8	0	1.622976	3.218844	0.000568

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.453902	0.000000			
3	C	1.422652	2.451731	0.000000		
4	C	2.438061	2.725464	1.444728	0.000000	
5	H	3.412448	3.813935	2.166276	1.088820	0.000000
6	C	3.188931	3.061539	2.750557	2.051863	2.483923
7	H	4.064169	3.772980	3.486413	2.390766	2.515460
8	C	2.920135	2.406067	3.146925	2.869735	3.635835
9	H	3.560300	2.614613	3.981918	3.570452	4.371018
10	C	1.416658	2.540942	2.440360	3.736551	4.598435
11	H	2.178262	2.805132	3.431685	4.613239	5.552131
12	C	2.430225	3.791113	2.795130	4.237563	4.857131
13	H	3.412534	4.676261	3.881492	5.323983	5.928590
14	C	2.821573	4.272858	2.420573	3.763124	4.090076
15	H	3.907824	5.359082	3.407328	4.650637	4.797158
16	C	2.457239	3.756937	1.410123	2.509437	2.713405
17	H	3.436744	4.611588	2.161231	2.743572	2.495323
18	C	2.850452	2.445707	2.466914	1.448054	2.174326
19	C	2.489029	1.455671	2.864416	2.447622	3.423090
20	C	3.778120	2.548396	4.261491	3.743554	4.606532
21	H	4.137702	2.796159	4.907347	4.607566	5.548562
22	C	4.880933	3.796329	5.060698	4.238373	4.859014
23	H	5.843641	4.683267	6.116553	5.325067	5.930283
24	C	5.076238	4.275238	4.852669	3.762004	4.090755
25	H	6.128817	5.361818	5.808825	4.647615	4.795203
26	C	4.241470	3.752432	3.724873	2.504145	2.712357
27	H	4.859915	4.605795	4.050954	2.734292	2.489116
28	C	3.117349	3.073595	3.481425	3.713082	4.414532
29	C	3.585505	3.957782	2.967721	2.768330	2.907619

30	O	3.434743	3.866747	3.295202	3.586782	3.999231
31	O	4.450845	4.998889	3.541277	3.286279	3.018379
32	O	3.685476	3.578385	4.359199	4.784230	5.555078
33	C	2.524541	1.491526	3.790831	4.180758	5.262650
34	H	2.683401	2.194434	4.024002	4.682383	5.732040
35	O	3.656293	2.415016	4.852441	5.028773	6.097950
		6	7	8	9	10
6	C	0.000000				
7	H	1.083803	0.000000			
8	C	1.413005	2.204927	0.000000		
9	H	2.233235	2.660424	1.081066	0.000000	
10	C	4.371301	5.338990	3.957050	4.596518	0.000000
11	H	5.061997	6.035334	4.376738	4.828796	1.084627
12	C	5.022307	5.986483	4.885228	5.684967	1.385442
13	H	6.032368	7.024386	5.797986	6.561382	2.140448
14	C	4.752421	5.607446	5.016037	5.948538	2.429853
15	H	5.628697	6.444352	5.987816	6.958092	3.408831
16	C	3.711599	4.432966	4.263322	5.211793	2.811237
17	H	3.980074	4.510226	4.823699	5.796569	3.897867
18	C	2.664811	2.716365	3.089388	3.361102	4.242407
19	C	3.117009	3.422259	2.859494	2.843420	3.768264
20	C	4.247952	4.338573	3.849434	3.452343	4.913810
21	H	4.924651	5.128250	4.242417	3.696136	5.062090
22	C	4.861951	4.650904	4.757941	4.342743	6.101514
23	H	5.862359	5.610302	5.660882	5.111857	6.994017
24	C	4.589006	4.166257	4.898509	4.695589	6.404185
25	H	5.457078	4.888582	5.866626	5.634312	7.455095
26	C	3.573349	3.192042	4.171771	4.264472	5.612756
27	H	3.858534	3.319267	4.749522	4.976893	6.207371
28	C	2.330556	3.299675	1.473581	2.225091	3.672023
29	C	1.494390	2.217130	2.325884	3.332421	4.428634
30	O	2.335222	3.284089	2.329405	3.314918	3.915578
31	O	2.443062	2.808515	3.500036	4.471705	5.219181
32	O	3.511449	4.446931	2.439542	2.833715	3.877205
33	C	4.079222	4.821578	2.978420	2.834610	2.979169
34	H	4.431006	5.318508	3.273665	3.315941	2.656778
35	O	4.848183	5.421708	3.690280	3.190989	4.139083
		11	12	13	14	15
11	H	0.000000				
12	C	2.135254	0.000000			
13	H	2.448318	1.086501	0.000000		
14	C	3.405771	1.409097	2.164271	0.000000	
15	H	4.293093	2.166087	2.489363	1.086303	0.000000
16	C	3.895526	2.419754	3.400381	1.384709	2.145968
17	H	4.982212	3.410664	4.305045	2.152344	2.483124
18	C	4.896909	5.048041	6.101281	4.846927	5.805851
19	C	4.135113	4.876545	5.835445	5.079396	6.133327
20	C	5.066465	6.106237	6.994761	6.416014	7.468822
21	H	4.980854	6.356649	7.139313	6.879752	7.950167
22	C	6.355894	7.191046	8.126342	7.315346	8.320673
23	H	7.141320	8.130151	9.023399	8.328704	9.338678
24	C	6.872635	7.308485	8.318061	7.158832	8.085553

25	H	7.940648	8.311117	9.325022	8.082509	8.963906
26	C	6.254393	6.360315	7.413773	6.033960	6.915375
27	H	6.964251	6.771624	7.840227	6.224659	6.993952
28	C	4.019458	4.414606	5.167961	4.668057	5.541928
29	C	5.213801	4.720852	5.643490	4.267206	4.958724
30	O	4.528461	4.233698	5.002055	4.113515	4.815079
31	O	6.103208	5.241807	6.131958	4.495302	4.969968
32	O	3.924734	4.661628	5.212723	5.197217	6.035908
33	C	2.681230	4.355675	5.003481	5.186702	6.247094
34	H	2.139735	3.950029	4.435051	4.951031	5.948536
35	O	3.720678	5.523691	6.123409	6.371164	7.435540

		16	17	18	19	20
16	C	0.000000				
17	H	1.086724	0.000000			
18	C	3.728828	4.064016	0.000000		
19	C	4.254997	4.879324	1.423238	0.000000	
20	C	5.632966	6.233268	2.441344	1.416522	0.000000
21	H	6.267673	6.982379	3.422727	2.164131	1.081533
22	C	6.375179	6.793728	2.793323	2.429335	1.387228
23	H	7.431675	7.865232	3.879971	3.411400	2.140796
24	C	6.042492	6.242157	2.421218	2.823224	2.433276
25	H	6.920723	7.008586	3.408084	3.909829	3.413008
26	C	4.824968	4.929045	1.408914	2.457270	2.813033
27	H	4.919097	4.780268	2.161159	3.437892	3.900664
28	C	4.248031	4.891083	4.282830	4.000201	5.070827
29	C	3.382875	3.522561	3.854077	4.355091	5.609203
30	O	3.649291	4.081374	4.569516	4.681397	5.924376
31	O	3.565637	3.349813	4.526706	5.276522	6.545728
32	O	5.054784	5.807091	5.243103	4.706098	5.636207
33	C	4.960852	5.905191	3.825503	2.582488	3.081483
34	H	4.977364	5.983195	4.620945	3.526046	4.172382
35	O	6.093981	7.002785	4.374143	2.990723	2.907107

		21	22	23	24	25
21	H	0.000000				
22	C	2.148041	0.000000			
23	H	2.467737	1.086760	0.000000		
24	C	3.414192	1.408548	2.163365	0.000000	
25	H	4.305924	2.167304	2.490289	1.086707	0.000000
26	C	3.894464	2.418469	3.399641	1.385977	2.147730
27	H	4.982064	3.410157	4.304994	2.153440	2.484210
28	C	5.310106	6.115824	7.010558	6.300712	7.291630
29	C	6.233113	6.292625	7.316115	5.959066	6.801709
30	O	6.338406	6.844425	7.827275	6.766878	7.704317
31	O	7.259985	7.089690	8.132770	6.554864	7.293850
32	O	5.655353	6.801772	7.610261	7.177663	8.195309
33	C	2.774799	4.460747	5.119801	5.274128	6.339644
34	H	3.862704	5.548060	6.222991	6.294948	7.371296
35	O	2.220189	4.223975	4.649415	5.288797	6.285765

		26	27	28	29	30
26	C	0.000000				
27	H	1.087678	0.000000			
28	C	5.489772	5.997996	0.000000		

29	C	4.810695	4.905054	2.279394	0.000000	
30	O	5.727975	6.003535	1.407122	1.387704	0.000000
31	O	5.301348	5.150863	3.419937	1.202599	2.269961
32	O	6.487574	7.084791	1.203449	3.411577	2.274304
33	C	5.017382	5.952010	3.308671	4.886659	4.438886
34	H	5.908713	6.771410	3.090917	4.928273	4.190308
35	O	5.345220	6.368027	4.201368	5.831860	5.447306

	31	32	33	34	35
31 O	0.000000				
32 O	4.483881	0.000000			
33 C	6.027670	3.307428	0.000000		
34 H	6.056703	2.769757	1.103232	0.000000	
35 O	6.995119	4.107412	1.220525	2.009994	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.521111	0.690914	1.078975
2	6	0	0.627209	1.131832	0.303873
3	6	0	-0.724137	-0.712953	1.187963
4	6	0	0.214432	-1.556153	0.484159
5	1	0	0.037637	-2.629717	0.525795
6	6	0	-0.257271	-1.194060	-1.479646
7	1	0	0.418878	-1.948160	-1.865372
8	6	0	-0.137332	0.183371	-1.770990
9	1	0	0.691557	0.667391	-2.268355
10	6	0	-1.453874	1.559271	1.697708
11	1	0	-1.316308	2.634408	1.658043
12	6	0	-2.529991	1.042312	2.400683
13	1	0	-3.223963	1.719855	2.890400
14	6	0	-2.733483	-0.349293	2.487753
15	1	0	-3.586788	-0.738630	3.035786
16	6	0	-1.847616	-1.218674	1.873885
17	1	0	-2.000808	-2.293325	1.925158
18	6	0	1.591785	-1.111652	0.437492
19	6	0	1.813944	0.288934	0.316613
20	6	0	3.143214	0.752930	0.160787
21	1	0	3.327614	1.813391	0.055286
22	6	0	4.198634	-0.147342	0.159822
23	1	0	5.215785	0.224577	0.069670
24	6	0	3.970418	-1.532683	0.272766
25	1	0	4.808705	-2.224193	0.268043
26	6	0	2.675138	-2.011257	0.391715
27	1	0	2.485277	-3.079141	0.473093
28	6	0	-1.498417	0.737282	-1.880854

Supplementary Material (ESI) for Green Chemistry
This journal is © The Royal Society of Chemistry 2014

```
   29          6             0       -1.720296   -1.498235   -1.495014
   30          8             0       -2.410506   -0.300126   -1.612768
   31          8             0       -2.283519   -2.556738   -1.402293
   32          8             0       -1.882040    1.846936   -2.145031
   33          6             0        0.660863    2.551875   -0.151095
   34          1             0       -0.324880    3.045504   -0.193048
   35          8             0        1.655394    3.156120   -0.519168
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3889907      0.2596874
0.2420784
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1906.9544560877 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1032.13801898     A.U. after   11 cycles
            Convg  =    0.7313D-08             -V/T =  2.0093
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000002030   -0.000000935   -0.000000477
    2          6          -0.000000370    0.000000903    0.000001817
    3          6           0.000000484   -0.000001034   -0.000000702
    4          6           0.000001178    0.000000428   -0.000002312
    5          1           0.000001814    0.000000483   -0.000001419
    6          6           0.000001750   -0.000000954    0.000001774
    7          1           0.000000731    0.000001485   -0.000000928
    8          6          -0.000002113    0.000000452   -0.000002245
    9          1           0.000000298    0.000002181    0.000001140
   10          6          -0.000000663   -0.000002156    0.000000906
   11          1          -0.000001352   -0.000001709    0.000001431
   12          6          -0.000000729   -0.000003172    0.000000316
   13          1          -0.000001082   -0.000003952    0.000000553
   14          6           0.000000309   -0.000003101   -0.000000415
   15          1           0.000000675   -0.000004065   -0.000000722
   16          6           0.000001132   -0.000002200   -0.000000912
   17          1           0.000001689   -0.000002245   -0.000001413
   18          6           0.000000759    0.000000455   -0.000000487
   19          6           0.000000061    0.000000312    0.000000394
   20          6           0.000000326    0.000001947    0.000001647
   21          1          -0.000001020    0.000001565    0.000000513
   22          6          -0.000000004    0.000002715    0.000000219
   23          1          -0.000000257    0.000003444    0.000000472
   24          6           0.000000765    0.000002855   -0.000000530
   25          1           0.000001452    0.000003337   -0.000000921
   26          6           0.000001521    0.000001845   -0.000000895
```

```
   27          1           0.000002143    0.000001678   -0.000001445
   28          6          -0.000000836    0.000000372    0.000000670
   29          6           0.000001039   -0.000000320   -0.000000426
   30          8          -0.000000110   -0.000000866   -0.000000165
   31          8           0.000001587   -0.000000912   -0.000001262
   32          8          -0.000001449   -0.000000203    0.000000907
   33          6          -0.000001317    0.000000356    0.000000743
   34          1          -0.000002708   -0.000000508    0.000002179
   35          8          -0.000003672    0.000001519    0.000001994
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000004065 RMS     0.000001547


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000001183 RMS     0.000000287
 Search for a saddle point.
 Step number  12 out of a maximum of 202
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Update second derivatives using D2CorX and points  4  5  6  7  8
                                                     9 10 11 12
     Eigenvalues ---   -0.01901   0.00217   0.00465   0.00671
0.00852
     Eigenvalues ---    0.00996   0.01264   0.01441   0.01484
0.01539
     Eigenvalues ---    0.01639   0.01668   0.01775   0.01876
0.01928
     Eigenvalues ---    0.01984   0.02131   0.02174   0.02189
0.02231
     Eigenvalues ---    0.02363   0.02426   0.02449   0.02518
0.02654
     Eigenvalues ---    0.02715   0.02746   0.02748   0.03001
0.03505
     Eigenvalues ---    0.03986   0.05546   0.07029   0.07378
0.07481
     Eigenvalues ---    0.08785   0.10166   0.11043   0.11179
0.11222
     Eigenvalues ---    0.11865   0.12276   0.12499   0.12527
0.12660
     Eigenvalues ---    0.12832   0.13904   0.14238   0.14641
0.16404
     Eigenvalues ---    0.17651   0.18495   0.19088   0.19170
0.19333
     Eigenvalues ---    0.19416   0.20108   0.20396   0.20896
0.21162
     Eigenvalues ---    0.23349   0.23905   0.24408   0.25102
0.26058
     Eigenvalues ---    0.27636   0.27927   0.29103   0.30148
0.30318
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.31236   0.33068   0.33990   0.34008
0.35003
     Eigenvalues ---    0.35269   0.35918   0.36086   0.36133
0.36201
     Eigenvalues ---    0.36237   0.36329   0.36536   0.37389
0.37812
     Eigenvalues ---    0.38851   0.39857   0.40317   0.41106
0.42459
     Eigenvalues ---    0.44476   0.46215   0.47305   0.47636
0.50256
     Eigenvalues ---    0.50615   0.79379   0.89039
0.902551000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
```

This journal is © The Royal Society of Chemistry 2014

1	-0.04212	0.02332	0.14747	0.01770	0.35431

	R6	R7	R8	R9	R10
1	0.09441	-0.04278	-0.02010	-0.06217	0.19897

	R11	R12	R13	R14	R15
1	0.01931	-0.00718	0.45447	0.19023	-0.05993

	R16	R17	R18	R19	R20
1	0.30082	-0.00776	-0.09479	0.18908	-0.01450

	R21	R22	R23	R24	R25
1	-0.02948	-0.00682	0.15116	-0.00454	-0.03917

	R26	R27	R28	R29	R30
1	0.06051	-0.00142	-0.01348	0.00008	0.01443

	R31	R32	R33	R34	R35
1	-0.00024	-0.01613	-0.00025	0.02105	0.01854

	R36	R37	R38	R39	R40
1	0.01756	-0.00150	-0.01216	-0.04481	0.00008

	R41	R42	R43	R44	R45
1	0.01318	-0.00013	-0.01557	-0.00014	0.00133

	R46	R47	R48	R49	R50
1	0.00070	-0.00083	0.00266	-0.00106	0.00488

	A1	A2	A3	A4	A5
1	0.02081	-0.00733	-0.01340	0.03126	-0.00395

	A6	A7	A8	A9	A10
1	0.00690	0.01908	-0.00127	-0.01661	0.03392

	A11	A12	A13	A14	A15
1	0.05742	0.03064	0.06368	0.04371	0.02353

	A16	A17	A18	A19	A20
1	0.04575	0.00648	0.01544	-0.00360	0.00685

	A21	A22	A23	A24	A25
1	-0.00333	-0.00142	0.00496	-0.00354	-0.00134

	A26	A27	A28	A29	A30
1	-0.00142	0.00276	0.00411	-0.00665	0.00246

	A31	A32	A33	A34	A35
1	0.01969	-0.01815	-0.00053	0.02071	-0.00706

	A36	A37	A38	A39	A40

This journal is © The Royal Society of Chemistry 2014

1	-0.01365	-0.00312	0.00705	-0.00394	-0.00114

	A41	A42	A43	A44	A45
1	0.00452	-0.00338	-0.00107	-0.00160	0.00266

	A46	A47	A48	A49	A50
1	0.00420	-0.00638	0.00209	-0.00233	0.00149

	A51	A52	A53	A54	A55
1	0.00084	-0.00677	0.00473	0.00213	-0.01365

	A56	A57	A58	D1	D2
1	-0.00112	0.00926	-0.00824	0.12917	-0.00243

	D3	D4	D5	D6	D7
1	0.12549	-0.00612	0.02271	0.00643	0.02622

	D8	D9	D10	D11	D12
1	0.00994	-0.00524	-0.00260	-0.00945	-0.00682

	D13	D14	D15	D16	D17
1	-0.13321	-0.13346	0.00301	0.00276	0.08577

	D18	D19	D20	D21	D22
1	0.08802	-0.05643	-0.05418	0.05574	-0.16104

	D23	D24	D25	D26	D27
1	0.07330	-0.14349	-0.00604	0.00058	-0.02509

	D28	D29	D30	D31	D32
1	-0.01847	0.15679	0.14482	-0.06215	-0.07411

	D33	D34	D35	D36	D37
1	0.02425	0.18116	-0.16581	-0.00890	-0.15475

	D38	D39	D40	D41	D42
1	-0.15972	0.03220	0.02723	-0.01653	-0.01485

	D43	D44	D45	D46	D47
1	0.13836	0.14005	-0.00139	-0.00063	0.00122

	D48	D49	D50	D51	D52
1	0.00198	0.00055	0.00480	0.00132	0.00557

	D53	D54	D55	D56	D57
1	-0.00141	-0.00819	0.00284	-0.00394	-0.01405

	D58	D59	D60	D61	D62
1	-0.01394	-0.00342	-0.00330	0.01515	0.01059

	D63	D64	D65	D66	D67

```
          1              0.00175  -0.00281   0.00266   0.00143
0.00332
                           D68       D69       D70       D71       D72
          1              0.00209   0.00222   0.00102   0.00098  -
0.00021
                           D73       D74       D75       D76       D77
          1              0.00078  -0.00250  -0.00043  -0.00370
0.00113
                           D78       D79       D80       D81       D82
          1              0.00586  -0.00215   0.00258   0.03920
0.03772
                           D83       D84
          1             -0.04664  -0.04206
 RFO step:  Lambda0=1.130974481D-11 Lambda= 0.00000000D+00.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.00002970 RMS(Int)=  0.00000000
 Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.74748   0.00000   0.00000  -0.00001  -0.00001
2.74747
    R2        2.68842   0.00000   0.00000   0.00000   0.00000
2.68842
    R3        5.51826   0.00000   0.00000   0.00010   0.00010
5.51836
    R4        2.67710   0.00000   0.00000   0.00000   0.00000
2.67710
    R5        4.54681   0.00000   0.00000   0.00019   0.00019
4.54700
    R6        4.94090   0.00000   0.00000   0.00011   0.00011
4.94101
    R7        2.75082   0.00000   0.00000  -0.00001  -0.00001
2.75081
    R8        2.81857   0.00000   0.00000   0.00000   0.00000
2.81857
    R9        2.73014   0.00000   0.00000   0.00000   0.00000
2.73015
   R10        5.19780   0.00000   0.00000  -0.00005  -0.00005
5.19775
   R11        2.66475   0.00000   0.00000   0.00000   0.00000
2.66475
   R12        2.05757   0.00000   0.00000   0.00000   0.00000
2.05757
   R13        3.87746   0.00000   0.00000  -0.00010  -0.00010
3.87736
   R14        4.51789   0.00000   0.00000  -0.00007  -0.00007
4.51782
   R15        2.73643   0.00000   0.00000   0.00000   0.00000
2.73643
   R16        4.69393   0.00000   0.00000  -0.00010  -0.00010
4.69383
```

This journal is © The Royal Society of Chemistry 2014

R17	2.04809	0.00000	0.00000	0.00000	0.00000
2.04809					
R18	2.67019	0.00000	0.00000	0.00000	0.00000
2.67019					
R19	5.03576	0.00000	0.00000	-0.00003	-0.00003
5.03574					
R20	2.82399	0.00000	0.00000	0.00001	0.00001
2.82400					
R21	5.13319	0.00000	0.00000	0.00001	0.00001
5.13319					
R22	2.04292	0.00000	0.00000	0.00000	0.00000
2.04292					
R23	5.40366	0.00000	0.00000	0.00011	0.00011
5.40377					
R24	2.78466	0.00000	0.00000	-0.00001	-0.00001
2.78465					
R25	5.37329	0.00000	0.00000	0.00003	0.00003
5.37332					
R26	5.35664	0.00000	0.00000	0.00011	0.00011
5.35675					
R27	2.04965	0.00000	0.00000	0.00000	0.00000
2.04965					
R28	2.61811	0.00000	0.00000	0.00000	0.00000
2.61810					
R29	2.05319	0.00000	0.00000	0.00000	0.00000
2.05319					
R30	2.66281	0.00000	0.00000	0.00000	0.00000
2.66281					
R31	2.05282	0.00000	0.00000	0.00000	0.00000
2.05282					
R32	2.61672	0.00000	0.00000	0.00000	0.00000
2.61672					
R33	2.05361	0.00000	0.00000	0.00000	0.00000
2.05361					
R34	2.68953	0.00000	0.00000	0.00000	0.00000
2.68953					
R35	2.66246	0.00000	0.00000	0.00000	0.00000
2.66246					
R36	2.67684	0.00000	0.00000	0.00000	0.00000
2.67684					
R37	2.04380	0.00000	0.00000	0.00000	0.00000
2.04380					
R38	2.62148	0.00000	0.00000	0.00000	0.00000
2.62148					
R39	4.19555	0.00000	0.00000	0.00005	0.00005
4.19560					
R40	2.05368	0.00000	0.00000	0.00000	0.00000
2.05368					
R41	2.66177	0.00000	0.00000	0.00000	0.00000
2.66177					
R42	2.05358	0.00000	0.00000	0.00000	0.00000
2.05358					

This journal is © The Royal Society of Chemistry 2014

R43	2.61912	0.00000	0.00000	0.00000	0.00000
2.61912					
R44	2.05541	0.00000	0.00000	0.00000	0.00000
2.05541					
R45	2.65907	0.00000	0.00000	0.00001	0.00001
2.65909					
R46	2.27419	0.00000	0.00000	0.00000	0.00000
2.27419					
R47	2.62238	0.00000	0.00000	-0.00001	-0.00001
2.62237					
R48	2.27258	0.00000	0.00000	0.00000	0.00000
2.27258					
R49	2.08481	0.00000	0.00000	0.00000	0.00000
2.08481					
R50	2.30646	0.00000	0.00000	0.00000	0.00000
2.30646					
A1	2.04072	0.00000	0.00000	0.00000	0.00000
2.04072					
A2	2.17364	0.00000	0.00000	-0.00001	-0.00001
2.17364					
A3	2.06854	0.00000	0.00000	0.00000	0.00000
2.06854					
A4	2.05288	0.00000	0.00000	0.00001	0.00001
2.05289					
A5	2.05915	0.00000	0.00000	0.00000	0.00000
2.05915					
A6	2.13598	0.00000	0.00000	0.00001	0.00001
2.13599					
A7	2.03298	0.00000	0.00000	0.00000	0.00000
2.03298					
A8	2.10002	0.00000	0.00000	0.00000	0.00000
2.10002					
A9	2.14747	0.00000	0.00000	0.00000	0.00000
2.14748					
A10	2.03907	0.00000	0.00000	-0.00001	-0.00001
2.03906					
A11	2.04258	0.00000	0.00000	0.00000	0.00000
2.04257					
A12	2.04692	0.00000	0.00000	-0.00001	-0.00001
2.04692					
A13	2.15548	0.00000	0.00000	-0.00001	-0.00001
2.15547					
A14	2.05498	0.00000	0.00000	-0.00001	-0.00001
2.05497					
A15	1.85397	0.00000	0.00000	-0.00001	-0.00001
1.85396					
A16	2.20980	0.00000	0.00000	0.00001	0.00001
2.20981					
A17	1.87906	0.00000	0.00000	0.00001	0.00001
1.87907					
A18	2.10087	0.00000	0.00000	0.00001	0.00001
2.10089					

This journal is © The Royal Society of Chemistry 2014

A19	2.10379	0.00000	0.00000	0.00000	0.00000
2.10379					
A20	2.09938	0.00000	0.00000	0.00000	0.00000
2.09938					
A21	2.07938	0.00000	0.00000	0.00000	0.00000
2.07938					
A22	2.08533	0.00000	0.00000	0.00000	0.00000
2.08533					
A23	2.10834	0.00000	0.00000	0.00000	0.00000
2.10834					
A24	2.08952	0.00000	0.00000	0.00000	0.00000
2.08952					
A25	2.09274	0.00000	0.00000	0.00000	0.00000
2.09274					
A26	2.09471	0.00000	0.00000	0.00000	0.00000
2.09471					
A27	2.09574	0.00000	0.00000	0.00000	0.00000
2.09574					
A28	2.09460	0.00000	0.00000	0.00000	0.00000
2.09460					
A29	2.08279	0.00000	0.00000	0.00000	0.00000
2.08279					
A30	2.10571	0.00000	0.00000	0.00000	0.00000
2.10571					
A31	2.04125	0.00000	0.00000	0.00000	0.00000
2.04125					
A32	2.13700	0.00000	0.00000	0.00000	0.00000
2.13700					
A33	2.10083	0.00000	0.00000	0.00000	0.00000
2.10083					
A34	2.03009	0.00000	0.00000	0.00000	0.00000
2.03009					
A35	2.18267	0.00000	0.00000	0.00000	0.00000
2.18266					
A36	2.06936	0.00000	0.00000	0.00000	0.00000
2.06937					
A37	2.08507	0.00000	0.00000	0.00000	0.00000
2.08507					
A38	2.09607	0.00000	0.00000	0.00000	0.00000
2.09607					
A39	2.10197	0.00000	0.00000	0.00000	0.00000
2.10197					
A40	2.08293	0.00000	0.00000	0.00000	0.00000
2.08294					
A41	2.11175	0.00000	0.00000	0.00000	0.00000
2.11175					
A42	2.08850	0.00000	0.00000	0.00000	0.00000
2.08850					
A43	2.09499	0.00000	0.00000	0.00000	0.00000
2.09499					
A44	2.09198	0.00000	0.00000	0.00000	0.00000
2.09198					

This journal is © The Royal Society of Chemistry 2014

A45	2.09621	0.00000	0.00000	0.00000	0.00000	2.09621
A46	2.09546	0.00000	0.00000	0.00000	0.00000	2.09546
A47	2.08316	0.00000	0.00000	0.00000	0.00000	2.08316
A48	2.10432	0.00000	0.00000	0.00000	0.00000	2.10432
A49	1.88323	0.00000	0.00000	0.00000	0.00000	1.88323
A50	2.28816	0.00000	0.00000	0.00001	0.00001	2.28816
A51	2.11179	0.00000	0.00000	0.00000	0.00000	2.11179
A52	1.88817	0.00000	0.00000	0.00000	0.00000	1.88817
A53	2.26123	0.00000	0.00000	-0.00001	-0.00001	2.26122
A54	2.13356	0.00000	0.00000	0.00000	0.00000	2.13357
A55	1.90742	0.00000	0.00000	0.00000	0.00000	1.90742
A56	2.00142	0.00000	0.00000	-0.00001	-0.00001	2.00141
A57	2.19164	0.00000	0.00000	0.00001	0.00001	2.19164
A58	2.08872	0.00000	0.00000	0.00000	0.00000	2.08873
D1	-0.56865	0.00000	0.00000	0.00003	0.00003	-0.56863
D2	2.84779	0.00000	0.00000	-0.00003	-0.00003	2.84776
D3	2.59899	0.00000	0.00000	0.00000	0.00000	2.59899
D4	-0.26775	0.00000	0.00000	-0.00006	-0.00006	-0.26781
D5	-0.02862	0.00000	0.00000	-0.00002	-0.00002	-0.02864
D6	-3.09353	0.00000	0.00000	-0.00002	-0.00002	-3.09354
D7	3.08855	0.00000	0.00000	0.00000	0.00000	3.08856
D8	0.02364	0.00000	0.00000	0.00001	0.00001	0.02365
D9	-0.05535	0.00000	0.00000	0.00001	0.00001	-0.05534
D10	3.12472	0.00000	0.00000	0.00002	0.00002	3.12474
D11	3.11268	0.00000	0.00000	-0.00002	-0.00002	3.11267
D12	0.00957	0.00000	0.00000	-0.00001	-0.00001	0.00956

This journal is © The Royal Society of Chemistry 2014

D13	0.56084	0.00000	0.00000	-0.00002	-0.00002	0.56082
D14	-2.63120	0.00000	0.00000	-0.00002	-0.00002	-2.63121
D15	-2.86851	0.00000	0.00000	0.00004	0.00004	-2.86848
D16	0.22263	0.00000	0.00000	0.00004	0.00004	0.22267
D17	-0.37882	0.00000	0.00000	0.00000	0.00000	-0.37882
D18	2.82033	0.00000	0.00000	-0.00001	-0.00001	2.82032
D19	3.05152	0.00000	0.00000	-0.00006	-0.00006	3.05145
D20	-0.03252	0.00000	0.00000	-0.00007	-0.00007	-0.03259
D21	-3.09382	0.00000	0.00000	-0.00002	-0.00002	-3.09385
D22	0.63100	0.00000	0.00000	0.00001	0.00001	0.63101
D23	-0.03120	0.00000	0.00000	-0.00003	-0.00003	-0.03122
D24	-2.58956	0.00000	0.00000	0.00001	0.00001	-2.58955
D25	-0.04159	0.00000	0.00000	0.00000	0.00000	-0.04160
D26	3.11392	0.00000	0.00000	0.00000	0.00000	3.11392
D27	-3.10130	0.00000	0.00000	0.00000	0.00000	-3.10130
D28	0.05422	0.00000	0.00000	0.00000	0.00000	0.05422
D29	-0.63848	0.00000	0.00000	-0.00001	-0.00001	-0.63849
D30	2.60016	0.00000	0.00000	0.00000	0.00000	2.60016
D31	3.08900	0.00000	0.00000	0.00003	0.00003	3.08902
D32	0.04445	0.00000	0.00000	0.00003	0.00003	0.04448
D33	-0.16980	0.00000	0.00000	-0.00011	-0.00011	-0.16991
D34	2.51534	0.00000	0.00000	-0.00002	-0.00002	2.51532
D35	-2.62568	0.00000	0.00000	-0.00007	-0.00007	-2.62575
D36	0.05946	0.00000	0.00000	0.00002	0.00002	0.05948
D37	-2.63577	0.00000	0.00000	0.00003	0.00003	-2.63574
D38	0.52849	0.00000	0.00000	0.00003	0.00003	0.52852

This journal is © The Royal Society of Chemistry 2014

D39	-0.13345	0.00000	0.00000	-0.00001	-0.00001	-0.13347
D40	3.03081	0.00000	0.00000	-0.00001	-0.00001	3.03080
D41	0.03245	0.00000	0.00000	-0.00002	-0.00002	0.03243
D42	-3.10711	0.00000	0.00000	-0.00002	-0.00002	-3.10712
D43	2.75151	0.00000	0.00000	0.00006	0.00006	2.75157
D44	-0.38805	0.00000	0.00000	0.00007	0.00007	-0.38799
D45	3.11582	0.00000	0.00000	0.00000	0.00000	3.11582
D46	-0.02529	0.00000	0.00000	0.00000	0.00000	-0.02529
D47	0.01217	0.00000	0.00000	0.00001	0.00001	0.01218
D48	-3.12894	0.00000	0.00000	0.00001	0.00001	-3.12893
D49	-3.13267	0.00000	0.00000	0.00000	0.00000	-3.13267
D50	0.00743	0.00000	0.00000	0.00000	0.00000	0.00743
D51	0.00940	0.00000	0.00000	0.00000	0.00000	0.00941
D52	-3.13368	0.00000	0.00000	0.00001	0.00001	-3.13368
D53	0.02603	0.00000	0.00000	0.00000	0.00000	0.02603
D54	-3.12967	0.00000	0.00000	0.00000	0.00000	-3.12967
D55	-3.11706	0.00000	0.00000	0.00000	0.00000	-3.11706
D56	0.01042	0.00000	0.00000	0.00000	0.00000	0.01043
D57	0.03943	0.00000	0.00000	0.00001	0.00001	0.03944
D58	-3.05515	0.00000	0.00000	0.00001	0.00001	-3.05514
D59	3.08610	0.00000	0.00000	0.00001	0.00001	3.08611
D60	-0.00847	0.00000	0.00000	0.00000	0.00000	-0.00847
D61	3.07865	0.00000	0.00000	-0.00001	-0.00001	3.07865
D62	-0.08681	0.00000	0.00000	-0.00001	-0.00001	-0.08682
D63	0.03733	0.00000	0.00000	0.00000	0.00000	0.03733
D64	-3.12814	0.00000	0.00000	0.00000	0.00000	-3.12814

This journal is © The Royal Society of Chemistry 2014

```
   D65        0.03832   0.00000   0.00000  -0.00002  -0.00002
0.03830
   D66       -3.11644   0.00000   0.00000  -0.00001  -0.00001  -
3.11645
   D67        3.12842   0.00000   0.00000  -0.00001  -0.00001
3.12842
   D68       -0.02633   0.00000   0.00000   0.00000   0.00000  -
0.02634
   D69       -3.10942   0.00000   0.00000   0.00000   0.00000  -
3.10942
   D70        0.03299   0.00000   0.00000   0.00000   0.00000
0.03299
   D71        0.01888   0.00000   0.00000   0.00001   0.00001
0.01888
   D72       -3.12190   0.00000   0.00000   0.00001   0.00001  -
3.12189
   D73        3.13918   0.00000   0.00000   0.00000   0.00000
3.13919
   D74       -0.00396   0.00000   0.00000   0.00000   0.00000  -
0.00396
   D75       -0.00159   0.00000   0.00000   0.00000   0.00000  -
0.00159
   D76        3.13845   0.00000   0.00000   0.00000   0.00000
3.13845
   D77       -0.03118   0.00000   0.00000   0.00000   0.00000  -
0.03119
   D78        3.13458   0.00000   0.00000   0.00000   0.00000
3.13457
   D79        3.10885   0.00000   0.00000   0.00000   0.00000
3.10885
   D80       -0.00857   0.00000   0.00000   0.00000   0.00000  -
0.00857
   D81       -0.11932   0.00000   0.00000   0.00001   0.00001  -
0.11931
   D82        3.02049   0.00000   0.00000   0.00001   0.00001
3.02049
   D83        0.15654   0.00000   0.00000   0.00000   0.00000
0.15654
   D84       -3.00572   0.00000   0.00000   0.00000   0.00000  -
3.00572
         Item               Value     Threshold  Converged?
 Maximum Force            0.000001     0.000450     YES
 RMS     Force            0.000000     0.000300     YES
 Maximum Displacement     0.000145     0.001800     YES
 RMS     Displacement     0.000030     0.001200     YES
 Predicted change in Energy=-3.713586D-10
 Optimization completed.
    -- Stationary point found.
                           ----------------------------
                           !   Optimized Parameters   !
                           ! (Angstroms and Degrees)  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ---------------------------                          ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ---------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.4539         -DE/DX =    0.0
!
 ! R2    R(1,3)                  1.4227         -DE/DX =    0.0
!
 ! R3    R(1,8)                  2.9201         -DE/DX =    0.0
!
 ! R4    R(1,10)                 1.4167         -DE/DX =    0.0
!
 ! R5    R(2,8)                  2.4061         -DE/DX =    0.0
!
 ! R6    R(2,9)                  2.6146         -DE/DX =    0.0
!
 ! R7    R(2,19)                 1.4557         -DE/DX =    0.0
!
 ! R8    R(2,33)                 1.4915         -DE/DX =    0.0
!
 ! R9    R(3,4)                  1.4447         -DE/DX =    0.0
!
 ! R10   R(3,6)                  2.7506         -DE/DX =    0.0
!
 ! R11   R(3,16)                 1.4101         -DE/DX =    0.0
!
 ! R12   R(4,5)                  1.0888         -DE/DX =    0.0
!
 ! R13   R(4,6)                  2.0519         -DE/DX =    0.0
!
 ! R14   R(4,7)                  2.3908         -DE/DX =    0.0
!
 ! R15   R(4,18)                 1.4481         -DE/DX =    0.0
!
 ! R16   R(5,6)                  2.4839         -DE/DX =    0.0
!
 ! R17   R(6,7)                  1.0838         -DE/DX =    0.0
!
 ! R18   R(6,8)                  1.413          -DE/DX =    0.0
!
 ! R19   R(6,18)                 2.6648         -DE/DX =    0.0
!
 ! R20   R(6,29)                 1.4944         -DE/DX =    0.0
!
 ! R21   R(7,18)                 2.7164         -DE/DX =    0.0
!
 ! R22   R(8,9)                  1.0811         -DE/DX =    0.0
!
 ! R23   R(8,19)                 2.8595         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R24   R(8,28)                 1.4736          -DE/DX =    0.0
!
 ! R25   R(9,19)                 2.8434          -DE/DX =    0.0
!
 ! R26   R(9,33)                 2.8346          -DE/DX =    0.0
!
 ! R27   R(10,11)                1.0846          -DE/DX =    0.0
!
 ! R28   R(10,12)                1.3854          -DE/DX =    0.0
!
 ! R29   R(12,13)                1.0865          -DE/DX =    0.0
!
 ! R30   R(12,14)                1.4091          -DE/DX =    0.0
!
 ! R31   R(14,15)                1.0863          -DE/DX =    0.0
!
 ! R32   R(14,16)                1.3847          -DE/DX =    0.0
!
 ! R33   R(16,17)                1.0867          -DE/DX =    0.0
!
 ! R34   R(18,19)                1.4232          -DE/DX =    0.0
!
 ! R35   R(18,26)                1.4089          -DE/DX =    0.0
!
 ! R36   R(19,20)                1.4165          -DE/DX =    0.0
!
 ! R37   R(20,21)                1.0815          -DE/DX =    0.0
!
 ! R38   R(20,22)                1.3872          -DE/DX =    0.0
!
 ! R39   R(21,35)                2.2202          -DE/DX =    0.0
!
 ! R40   R(22,23)                1.0868          -DE/DX =    0.0
!
 ! R41   R(22,24)                1.4085          -DE/DX =    0.0
!
 ! R42   R(24,25)                1.0867          -DE/DX =    0.0
!
 ! R43   R(24,26)                1.386           -DE/DX =    0.0
!
 ! R44   R(26,27)                1.0877          -DE/DX =    0.0
!
 ! R45   R(28,30)                1.4071          -DE/DX =    0.0
!
 ! R46   R(28,32)                1.2034          -DE/DX =    0.0
!
 ! R47   R(29,30)                1.3877          -DE/DX =    0.0
!
 ! R48   R(29,31)                1.2026          -DE/DX =    0.0
!
 ! R49   R(33,34)                1.1032          -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R50   R(33,35)                1.2205         -DE/DX =    0.0
!
 ! A1    A(2,1,3)              116.9246         -DE/DX =    0.0
!
 ! A2    A(2,1,10)             124.5405         -DE/DX =    0.0
!
 ! A3    A(3,1,10)             118.5186         -DE/DX =    0.0
!
 ! A4    A(1,2,19)             117.6216         -DE/DX =    0.0
!
 ! A5    A(1,2,33)             117.9806         -DE/DX =    0.0
!
 ! A6    A(19,2,33)            122.3824         -DE/DX =    0.0
!
 ! A7    A(1,3,4)              116.481          -DE/DX =    0.0
!
 ! A8    A(1,3,16)             120.3224         -DE/DX =    0.0
!
 ! A9    A(4,3,16)             123.0412         -DE/DX =    0.0
!
 ! A10   A(3,4,5)              116.8302         -DE/DX =    0.0
!
 ! A11   A(3,4,18)             117.0312         -DE/DX =    0.0
!
 ! A12   A(5,4,18)             117.2801         -DE/DX =    0.0
!
 ! A13   A(7,6,8)              123.4999         -DE/DX =    0.0
!
 ! A14   A(7,6,29)             117.7419         -DE/DX =    0.0
!
 ! A15   A(8,6,29)             106.2244         -DE/DX =    0.0
!
 ! A16   A(6,8,9)              126.6122         -DE/DX =    0.0
!
 ! A17   A(6,8,28)             107.662          -DE/DX =    0.0
!
 ! A18   A(9,8,28)             120.3713         -DE/DX =    0.0
!
 ! A19   A(1,10,11)            120.5384         -DE/DX =    0.0
!
 ! A20   A(1,10,12)            120.2856         -DE/DX =    0.0
!
 ! A21   A(11,10,12)           119.1398         -DE/DX =    0.0
!
 ! A22   A(10,12,13)           119.4805         -DE/DX =    0.0
!
 ! A23   A(10,12,14)           120.799          -DE/DX =    0.0
!
 ! A24   A(13,12,14)           119.7205         -DE/DX =    0.0
!
 ! A25   A(12,14,15)           119.9053         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A26   A(12,14,16)           120.0178         -DE/DX =    0.0
!
 ! A27   A(15,14,16)           120.0768         -DE/DX =    0.0
!
 ! A28   A(3,16,14)            120.0118         -DE/DX =    0.0
!
 ! A29   A(3,16,17)            119.3349         -DE/DX =    0.0
!
 ! A30   A(14,16,17)           120.6484         -DE/DX =    0.0
!
 ! A31   A(4,18,19)            116.9549         -DE/DX =    0.0
!
 ! A32   A(4,18,26)            122.4411         -DE/DX =    0.0
!
 ! A33   A(19,18,26)           120.3687         -DE/DX =    0.0
!
 ! A34   A(2,19,18)            116.3157         -DE/DX =    0.0
!
 ! A35   A(2,19,20)            125.0575         -DE/DX =    0.0
!
 ! A36   A(18,19,20)           118.5659         -DE/DX =    0.0
!
 ! A37   A(19,20,21)           119.4659         -DE/DX =    0.0
!
 ! A38   A(19,20,22)           120.0959         -DE/DX =    0.0
!
 ! A39   A(21,20,22)           120.4338         -DE/DX =    0.0
!
 ! A40   A(20,22,23)           119.3433         -DE/DX =    0.0
!
 ! A41   A(20,22,24)           120.9945         -DE/DX =    0.0
!
 ! A42   A(23,22,24)           119.6622         -DE/DX =    0.0
!
 ! A43   A(22,24,25)           120.0343         -DE/DX =    0.0
!
 ! A44   A(22,24,26)           119.8618         -DE/DX =    0.0
!
 ! A45   A(25,24,26)           120.1039         -DE/DX =    0.0
!
 ! A46   A(18,26,24)           120.0611         -DE/DX =    0.0
!
 ! A47   A(18,26,27)           119.3562         -DE/DX =    0.0
!
 ! A48   A(24,26,27)           120.5685         -DE/DX =    0.0
!
 ! A49   A(8,28,30)            107.9012         -DE/DX =    0.0
!
 ! A50   A(8,28,32)            131.1018         -DE/DX =    0.0
!
 ! A51   A(30,28,32)           120.9969         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A52   A(6,29,30)            108.1842         -DE/DX =    0.0
!
 ! A53   A(6,29,31)            129.5589         -DE/DX =    0.0
!
 ! A54   A(30,29,31)           122.2441         -DE/DX =    0.0
!
 ! A55   A(28,30,29)           109.2869         -DE/DX =    0.0
!
 ! A56   A(2,33,34)            114.6727         -DE/DX =    0.0
!
 ! A57   A(2,33,35)            125.5715         -DE/DX =    0.0
!
 ! A58   A(34,33,35)           119.6751         -DE/DX =    0.0
!
 ! D1    D(3,1,2,19)            -32.5814         -DE/DX =    0.0
!
 ! D2    D(3,1,2,33)            163.1663         -DE/DX =    0.0
!
 ! D3    D(10,1,2,19)           148.9114         -DE/DX =    0.0
!
 ! D4    D(10,1,2,33)           -15.3409         -DE/DX =    0.0
!
 ! D5    D(2,1,3,4)              -1.6396         -DE/DX =    0.0
!
 ! D6    D(2,1,3,16)           -177.246          -DE/DX =    0.0
!
 ! D7    D(10,1,3,4)            176.9609         -DE/DX =    0.0
!
 ! D8    D(10,1,3,16)             1.3546         -DE/DX =    0.0
!
 ! D9    D(2,1,10,11)            -3.1712         -DE/DX =    0.0
!
 ! D10   D(2,1,10,12)           179.0335         -DE/DX =    0.0
!
 ! D11   D(3,1,10,11)           178.3436         -DE/DX =    0.0
!
 ! D12   D(3,1,10,12)             0.5483         -DE/DX =    0.0
!
 ! D13   D(1,2,19,18)            32.134          -DE/DX =    0.0
!
 ! D14   D(1,2,19,20)          -150.7565         -DE/DX =    0.0
!
 ! D15   D(33,2,19,18)         -164.3537         -DE/DX =    0.0
!
 ! D16   D(33,2,19,20)           12.7557         -DE/DX =    0.0
!
 ! D17   D(1,2,33,34)           -21.7048         -DE/DX =    0.0
!
 ! D18   D(1,2,33,35)           161.5928         -DE/DX =    0.0
!
 ! D19   D(19,2,33,34)          174.8391         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D20   D(19,2,33,35)          -1.8633         -DE/DX =    0.0
!
 ! D21   D(1,3,4,5)            -177.263          -DE/DX =    0.0
!
 ! D22   D(1,3,4,18)             36.1536         -DE/DX =    0.0
!
 ! D23   D(16,3,4,5)             -1.7875         -DE/DX =    0.0
!
 ! D24   D(16,3,4,18)          -148.3709         -DE/DX =    0.0
!
 ! D25   D(1,3,16,14)            -2.3832         -DE/DX =    0.0
!
 ! D26   D(1,3,16,17)           178.4143         -DE/DX =    0.0
!
 ! D27   D(4,3,16,14)          -177.6912         -DE/DX =    0.0
!
 ! D28   D(4,3,16,17)             3.1063         -DE/DX =    0.0
!
 ! D29   D(3,4,18,19)           -36.5822         -DE/DX =    0.0
!
 ! D30   D(3,4,18,26)           148.978          -DE/DX =    0.0
!
 ! D31   D(5,4,18,19)           176.9865         -DE/DX =    0.0
!
 ! D32   D(5,4,18,26)             2.5466         -DE/DX =    0.0
!
 ! D33   D(7,6,8,9)              -9.7286         -DE/DX =    0.0
!
 ! D34   D(7,6,8,28)            144.1184         -DE/DX =    0.0
!
 ! D35   D(29,6,8,9)           -150.4403         -DE/DX =    0.0
!
 ! D36   D(29,6,8,28)             3.4066         -DE/DX =    0.0
!
 ! D37   D(7,6,29,30)          -151.0186         -DE/DX =    0.0
!
 ! D38   D(7,6,29,31)            30.2804         -DE/DX =    0.0
!
 ! D39   D(8,6,29,30)            -7.6464         -DE/DX =    0.0
!
 ! D40   D(8,6,29,31)           173.6526         -DE/DX =    0.0
!
 ! D41   D(6,8,28,30)             1.8595         -DE/DX =    0.0
!
 ! D42   D(6,8,28,32)          -178.024          -DE/DX =    0.0
!
 ! D43   D(9,8,28,30)           157.6497         -DE/DX =    0.0
!
 ! D44   D(9,8,28,32)           -22.2338         -DE/DX =    0.0
!
 ! D45   D(1,10,12,13)          178.5234         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D46   D(1,10,12,14)          -1.4491         -DE/DX =    0.0
!
 ! D47   D(11,10,12,13)          0.6974         -DE/DX =    0.0
!
 ! D48   D(11,10,12,14)       -179.2751         -DE/DX =    0.0
!
 ! D49   D(10,12,14,15)       -179.4887         -DE/DX =    0.0
!
 ! D50   D(10,12,14,16)          0.4256         -DE/DX =    0.0
!
 ! D51   D(13,12,14,15)          0.5388         -DE/DX =    0.0
!
 ! D52   D(13,12,14,16)       -179.5469         -DE/DX =    0.0
!
 ! D53   D(12,14,16,3)           1.4913         -DE/DX =    0.0
!
 ! D54   D(12,14,16,17)       -179.3169         -DE/DX =    0.0
!
 ! D55   D(15,14,16,3)        -178.5946         -DE/DX =    0.0
!
 ! D56   D(15,14,16,17)          0.5973         -DE/DX =    0.0
!
 ! D57   D(4,18,19,2)            2.2589         -DE/DX =    0.0
!
 ! D58   D(4,18,19,20)        -175.0472         -DE/DX =    0.0
!
 ! D59   D(26,18,19,2)         176.8206         -DE/DX =    0.0
!
 ! D60   D(26,18,19,20)         -0.4855         -DE/DX =    0.0
!
 ! D61   D(4,18,26,24)         176.3938         -DE/DX =    0.0
!
 ! D62   D(4,18,26,27)          -4.9741         -DE/DX =    0.0
!
 ! D63   D(19,18,26,24)          2.1386         -DE/DX =    0.0
!
 ! D64   D(19,18,26,27)       -179.2292         -DE/DX =    0.0
!
 ! D65   D(2,19,20,21)           2.1956         -DE/DX =    0.0
!
 ! D66   D(2,19,20,22)        -178.5587         -DE/DX =    0.0
!
 ! D67   D(18,19,20,21)        179.2455         -DE/DX =    0.0
!
 ! D68   D(18,19,20,22)         -1.5088         -DE/DX =    0.0
!
 ! D69   D(19,20,22,23)       -178.1568         -DE/DX =    0.0
!
 ! D70   D(19,20,22,24)          1.89           -DE/DX =    0.0
!
 ! D71   D(21,20,22,23)          1.0815         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D72   D(21,20,22,24)       -178.8717         -DE/DX =    0.0
!
 ! D73   D(20,22,24,25)        179.862          -DE/DX =    0.0
!
 ! D74   D(20,22,24,26)         -0.227          -DE/DX =    0.0
!
 ! D75   D(23,22,24,25)         -0.0911         -DE/DX =    0.0
!
 ! D76   D(23,22,24,26)        179.82           -DE/DX =    0.0
!
 ! D77   D(22,24,26,18)         -1.7867         -DE/DX =    0.0
!
 ! D78   D(22,24,26,27)        179.598          -DE/DX =    0.0
!
 ! D79   D(25,24,26,18)        178.1243         -DE/DX =    0.0
!
 ! D80   D(25,24,26,27)         -0.4911         -DE/DX =    0.0
!
 ! D81   D(8,28,30,29)          -6.8366         -DE/DX =    0.0
!
 ! D82   D(32,28,30,29)        173.0611         -DE/DX =    0.0
!
 ! D83   D(6,29,30,28)           8.969          -DE/DX =    0.0
!
 ! D84   D(31,29,30,28)       -172.215          -DE/DX =    0.0
!
 ---------------------------------------------------------------------
-----------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.556113    0.522802    1.163068
    2          6             0        0.604236    1.084877    0.491137
    3          6             0       -0.741590   -0.883932    1.059931
    4          6             0        0.225759   -1.604686    0.264955
    5          1             0        0.063405   -2.674549    0.144277
    6          6             0       -0.203307   -0.963299   -1.636273
    7          1             0        0.492734   -1.645395   -2.110509
    8          6             0       -0.096082    0.443172   -1.719503
    9          1             0        0.737608    1.003723   -2.118812
   10          6             0       -1.515956    1.280988    1.877755
   11          1             0       -1.392886    2.351701    1.999589
   12          6             0       -2.601292    0.655053    2.469110
   13          1             0       -3.316575    1.245974    3.034503
   14          6             0       -2.786878   -0.736341    2.346083
   15          1             0       -3.647561   -1.210936    2.808727
```

16	6	0	-1.874016	-1.496751	1.634832
17	1	0	-2.012995	-2.568853	1.524141
18	6	0	1.597330	-1.143555	0.319853
19	6	0	1.802266	0.261882	0.411251
20	6	0	3.128142	0.757808	0.359806
21	1	0	3.299835	1.824166	0.415609
22	6	0	4.196064	-0.121318	0.254537
23	1	0	5.209670	0.270581	0.246405
24	6	0	3.985047	-1.510576	0.157369
25	1	0	4.833022	-2.184965	0.073295
26	6	0	2.694251	-2.015147	0.171099
27	1	0	2.517791	-3.085364	0.090212
28	6	0	-1.461898	0.992730	-1.782536
29	6	0	-1.661021	-1.277436	-1.734200
30	8	0	-2.365266	-0.082413	-1.693177
31	8	0	-2.211104	-2.344001	-1.812240
32	8	0	-1.854859	2.125007	-1.891262
33	6	0	0.628568	2.556595	0.250093
34	1	0	-0.362838	3.040545	0.255181
35	8	0	1.622976	3.218844	0.000568

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.453902	0.000000			
3	C	1.422652	2.451731	0.000000		
4	C	2.438061	2.725464	1.444728	0.000000	
5	H	3.412448	3.813935	2.166276	1.088820	0.000000
6	C	3.188931	3.061539	2.750557	2.051863	2.483923
7	H	4.064169	3.772980	3.486413	2.390766	2.515460
8	C	2.920135	2.406067	3.146925	2.869735	3.635835
9	H	3.560300	2.614613	3.981918	3.570452	4.371018
10	C	1.416658	2.540942	2.440360	3.736551	4.598435
11	H	2.178262	2.805132	3.431685	4.613239	5.552131
12	C	2.430225	3.791113	2.795130	4.237563	4.857131
13	H	3.412534	4.676261	3.881492	5.323983	5.928590
14	C	2.821573	4.272858	2.420573	3.763124	4.090076
15	H	3.907824	5.359082	3.407328	4.650637	4.797158
16	C	2.457239	3.756937	1.410123	2.509437	2.713405
17	H	3.436744	4.611588	2.161231	2.743572	2.495323
18	C	2.850452	2.445707	2.466914	1.448054	2.174326
19	C	2.489029	1.455671	2.864416	2.447622	3.423090
20	C	3.778120	2.548396	4.261491	3.743554	4.606532
21	H	4.137702	2.796159	4.907347	4.607566	5.548562
22	C	4.880933	3.796329	5.060698	4.238373	4.859014
23	H	5.843641	4.683267	6.116553	5.325067	5.930283
24	C	5.076238	4.275238	4.852669	3.762004	4.090755
25	H	6.128817	5.361818	5.808825	4.647615	4.795203
26	C	4.241470	3.752432	3.724873	2.504145	2.712357
27	H	4.859915	4.605795	4.050954	2.734292	2.489116
28	C	3.117349	3.073595	3.481425	3.713082	4.414532
29	C	3.585505	3.957782	2.967721	2.768330	2.907619

30	O	3.434743	3.866747	3.295202	3.586782	3.999231
31	O	4.450845	4.998889	3.541277	3.286279	3.018379
32	O	3.685476	3.578385	4.359199	4.784230	5.555078
33	C	2.524541	1.491526	3.790831	4.180758	5.262650
34	H	2.683401	2.194434	4.024002	4.682383	5.732040
35	O	3.656293	2.415016	4.852441	5.028773	6.097950
		6	7	8	9	10
6	C	0.000000				
7	H	1.083803	0.000000			
8	C	1.413005	2.204927	0.000000		
9	H	2.233235	2.660424	1.081066	0.000000	
10	C	4.371301	5.338990	3.957050	4.596518	0.000000
11	H	5.061997	6.035334	4.376738	4.828796	1.084627
12	C	5.022307	5.986483	4.885228	5.684967	1.385442
13	H	6.032368	7.024386	5.797986	6.561382	2.140448
14	C	4.752421	5.607446	5.016037	5.948538	2.429853
15	H	5.628697	6.444352	5.987816	6.958092	3.408831
16	C	3.711599	4.432966	4.263322	5.211793	2.811237
17	H	3.980074	4.510226	4.823699	5.796569	3.897867
18	C	2.664811	2.716365	3.089388	3.361102	4.242407
19	C	3.117009	3.422259	2.859494	2.843420	3.768264
20	C	4.247952	4.338573	3.849434	3.452343	4.913810
21	H	4.924651	5.128250	4.242417	3.696136	5.062090
22	C	4.861951	4.650904	4.757941	4.342743	6.101514
23	H	5.862359	5.610302	5.660882	5.111857	6.994017
24	C	4.589006	4.166257	4.898509	4.695589	6.404185
25	H	5.457078	4.888582	5.866626	5.634312	7.455095
26	C	3.573349	3.192042	4.171771	4.264472	5.612756
27	H	3.858534	3.319267	4.749522	4.976893	6.207371
28	C	2.330556	3.299675	1.473581	2.225091	3.672023
29	C	1.494390	2.217130	2.325884	3.332421	4.428634
30	O	2.335222	3.284089	2.329405	3.314918	3.915578
31	O	2.443062	2.808515	3.500036	4.471705	5.219181
32	O	3.511449	4.446931	2.439542	2.833715	3.877205
33	C	4.079222	4.821578	2.978420	2.834610	2.979169
34	H	4.431006	5.318508	3.273665	3.315941	2.656778
35	O	4.848183	5.421708	3.690280	3.190989	4.139083
		11	12	13	14	15
11	H	0.000000				
12	C	2.135254	0.000000			
13	H	2.448318	1.086501	0.000000		
14	C	3.405771	1.409097	2.164271	0.000000	
15	H	4.293093	2.166087	2.489363	1.086303	0.000000
16	C	3.895526	2.419754	3.400381	1.384709	2.145968
17	H	4.982212	3.410664	4.305045	2.152344	2.483124
18	C	4.896909	5.048041	6.101281	4.846927	5.805851
19	C	4.135113	4.876545	5.835445	5.079396	6.133327
20	C	5.066465	6.106237	6.994761	6.416014	7.468822
21	H	4.980854	6.356649	7.139313	6.879752	7.950167
22	C	6.355894	7.191046	8.126342	7.315346	8.320673
23	H	7.141320	8.130151	9.023399	8.328704	9.338678
24	C	6.872635	7.308485	8.318061	7.158832	8.085553

This journal is © The Royal Society of Chemistry 2014

25	H	7.940648	8.311117	9.325022	8.082509	8.963906
26	C	6.254393	6.360315	7.413773	6.033960	6.915375
27	H	6.964251	6.771624	7.840227	6.224659	6.993952
28	C	4.019458	4.414606	5.167961	4.668057	5.541928
29	C	5.213801	4.720852	5.643490	4.267206	4.958724
30	O	4.528461	4.233698	5.002055	4.113515	4.815079
31	O	6.103208	5.241807	6.131958	4.495302	4.969968
32	O	3.924734	4.661628	5.212723	5.197217	6.035908
33	C	2.681230	4.355675	5.003481	5.186702	6.247094
34	H	2.139735	3.950029	4.435051	4.951031	5.948536
35	O	3.720678	5.523691	6.123409	6.371164	7.435540

		16	17	18	19	20
16	C	0.000000				
17	H	1.086724	0.000000			
18	C	3.728828	4.064016	0.000000		
19	C	4.254997	4.879324	1.423238	0.000000	
20	C	5.632966	6.233268	2.441344	1.416522	0.000000
21	H	6.267673	6.982379	3.422727	2.164131	1.081533
22	C	6.375179	6.793728	2.793323	2.429335	1.387228
23	H	7.431675	7.865232	3.879971	3.411400	2.140796
24	C	6.042492	6.242157	2.421218	2.823224	2.433276
25	H	6.920723	7.008586	3.408084	3.909829	3.413008
26	C	4.824968	4.929045	1.408914	2.457270	2.813033
27	H	4.919097	4.780268	2.161159	3.437892	3.900664
28	C	4.248031	4.891083	4.282830	4.000201	5.070827
29	C	3.382875	3.522561	3.854077	4.355091	5.609203
30	O	3.649291	4.081374	4.569516	4.681397	5.924376
31	O	3.565637	3.349813	4.526706	5.276522	6.545728
32	O	5.054784	5.807091	5.243103	4.706098	5.636207
33	C	4.960852	5.905191	3.825503	2.582488	3.081483
34	H	4.977364	5.983195	4.620945	3.526046	4.172382
35	O	6.093981	7.002785	4.374143	2.990723	2.907107

		21	22	23	24	25
21	H	0.000000				
22	C	2.148041	0.000000			
23	H	2.467737	1.086760	0.000000		
24	C	3.414192	1.408548	2.163365	0.000000	
25	H	4.305924	2.167304	2.490289	1.086707	0.000000
26	C	3.894464	2.418469	3.399641	1.385977	2.147730
27	H	4.982064	3.410157	4.304994	2.153440	2.484210
28	C	5.310106	6.115824	7.010558	6.300712	7.291630
29	C	6.233113	6.292625	7.316115	5.959066	6.801709
30	O	6.338406	6.844425	7.827275	6.766878	7.704317
31	O	7.259985	7.089690	8.132770	6.554864	7.293850
32	O	5.655353	6.801772	7.610261	7.177663	8.195309
33	C	2.774799	4.460747	5.119801	5.274128	6.339644
34	H	3.862704	5.548060	6.222991	6.294948	7.371296
35	O	2.220189	4.223975	4.649415	5.288797	6.285765

		26	27	28	29	30
26	C	0.000000				
27	H	1.087678	0.000000			
28	C	5.489772	5.997996	0.000000		

This journal is © The Royal Society of Chemistry 2014

29	C	4.810695	4.905054	2.279394	0.000000	
30	O	5.727975	6.003535	1.407122	1.387704	0.000000
31	O	5.301348	5.150863	3.419937	1.202599	2.269961
32	O	6.487574	7.084791	1.203449	3.411577	2.274304
33	C	5.017382	5.952010	3.308671	4.886659	4.438886
34	H	5.908713	6.771410	3.090917	4.928273	4.190308
35	O	5.345220	6.368027	4.201368	5.831860	5.447306

	31	32	33	34	35
31 O	0.000000				
32 O	4.483881	0.000000			
33 C	6.027670	3.307428	0.000000		
34 H	6.056703	2.769757	1.103232	0.000000	
35 O	6.995119	4.107412	1.220525	2.009994	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.521111	0.690914	1.078975
2	6	0	0.627209	1.131832	0.303873
3	6	0	-0.724137	-0.712953	1.187963
4	6	0	0.214432	-1.556153	0.484159
5	1	0	0.037637	-2.629717	0.525795
6	6	0	-0.257271	-1.194060	-1.479646
7	1	0	0.418878	-1.948160	-1.865372
8	6	0	-0.137332	0.183371	-1.770990
9	1	0	0.691557	0.667391	-2.268355
10	6	0	-1.453874	1.559271	1.697708
11	1	0	-1.316308	2.634408	1.658043
12	6	0	-2.529991	1.042312	2.400683
13	1	0	-3.223963	1.719855	2.890400
14	6	0	-2.733483	-0.349293	2.487753
15	1	0	-3.586788	-0.738630	3.035786
16	6	0	-1.847616	-1.218674	1.873885
17	1	0	-2.000808	-2.293325	1.925158
18	6	0	1.591785	-1.111652	0.437492
19	6	0	1.813944	0.288934	0.316613
20	6	0	3.143214	0.752930	0.160787
21	1	0	3.327614	1.813391	0.055286
22	6	0	4.198634	-0.147342	0.159822
23	1	0	5.215785	0.224577	0.069670
24	6	0	3.970418	-1.532683	0.272766
25	1	0	4.808705	-2.224193	0.268043
26	6	0	2.675138	-2.011257	0.391715
27	1	0	2.485277	-3.079141	0.473093
28	6	0	-1.498417	0.737282	-1.880854

This journal is © The Royal Society of Chemistry 2014

```
   29          6             0        -1.720296   -1.498235   -1.495014
   30          8             0        -2.410506   -0.300126   -1.612768
   31          8             0        -2.283519   -2.556738   -1.402293
   32          8             0        -1.882040    1.846936   -2.145031
   33          6             0         0.660863    2.551875   -0.151095
   34          1             0        -0.324880    3.045504   -0.193048
   35          8             0         1.655394    3.156120   -0.519168
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3889907      0.2596874
0.2420784


**********************************************************************

            Population analysis using the SCF density.

**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.22864 -19.17630 -19.17406 -19.17334 -
10.34953
 Alpha  occ. eigenvalues --  -10.34628 -10.29871 -10.25975 -10.25705 -
10.25210
 Alpha  occ. eigenvalues --  -10.24639 -10.23921 -10.23666 -10.23517 -
10.23446
 Alpha  occ. eigenvalues --  -10.22403 -10.22360 -10.22317 -10.22227 -
10.22157
 Alpha  occ. eigenvalues --  -10.22074 -10.21969 -10.21587  -1.14771
-1.08348
 Alpha  occ. eigenvalues --   -1.06664  -1.04510  -0.92368  -0.88335
-0.84949
 Alpha  occ. eigenvalues --   -0.82965  -0.82078  -0.78044  -0.77368
-0.74412
 Alpha  occ. eigenvalues --   -0.70910  -0.69157  -0.66480  -0.64262
-0.63920
 Alpha  occ. eigenvalues --   -0.62551  -0.59880  -0.59105  -0.57020
-0.55183
 Alpha  occ. eigenvalues --   -0.53182  -0.51659  -0.50801  -0.49980
-0.49429
 Alpha  occ. eigenvalues --   -0.49053  -0.48190  -0.47670  -0.46751
-0.46186
 Alpha  occ. eigenvalues --   -0.45168  -0.44940  -0.44513  -0.44292
-0.43750
 Alpha  occ. eigenvalues --   -0.42546  -0.42323  -0.41241  -0.40731
-0.40247
 Alpha  occ. eigenvalues --   -0.38962  -0.37699  -0.37229  -0.36741
-0.35983
 Alpha  occ. eigenvalues --   -0.33975  -0.32617  -0.32168  -0.29687
-0.28288
 Alpha  occ. eigenvalues --   -0.27858  -0.27634  -0.27279  -0.24622
 Alpha virt. eigenvalues --   -0.12605  -0.08338  -0.05184  -0.04147
-0.03321
 Alpha virt. eigenvalues --   -0.01418  -0.00884  -0.00068   0.00707
0.00768
 Alpha virt. eigenvalues --    0.01029   0.01982   0.02237   0.03218
0.03380
 Alpha virt. eigenvalues --    0.03779   0.03950   0.04470   0.04532
0.05780
 Alpha virt. eigenvalues --    0.06047   0.06250   0.06475   0.06967
0.07703
 Alpha virt. eigenvalues --    0.08069   0.08297   0.08721   0.09512
0.09898
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.10123   0.10454   0.10996   0.11356
0.11518
 Alpha virt. eigenvalues --    0.12215   0.12417   0.12618   0.13192
0.13646
 Alpha virt. eigenvalues --    0.13730   0.14032   0.14216   0.14607
0.15312
 Alpha virt. eigenvalues --    0.15499   0.15868   0.16056   0.16216
0.16410
 Alpha virt. eigenvalues --    0.16843   0.17205   0.17459   0.18158
0.18303
 Alpha virt. eigenvalues --    0.18629   0.18914   0.19376   0.19378
0.19445
 Alpha virt. eigenvalues --    0.20017   0.20129   0.20568   0.20866
0.21250
 Alpha virt. eigenvalues --    0.21920   0.21973   0.22401   0.22716
0.22889
 Alpha virt. eigenvalues --    0.23014   0.23322   0.23634   0.23860
0.24296
 Alpha virt. eigenvalues --    0.24740   0.24961   0.25158   0.25388
0.25858
 Alpha virt. eigenvalues --    0.25903   0.26278   0.26785   0.27337
0.27532
 Alpha virt. eigenvalues --    0.27978   0.28329   0.28548   0.28611
0.29101
 Alpha virt. eigenvalues --    0.29244   0.29474   0.29922   0.30378
0.30709
 Alpha virt. eigenvalues --    0.31263   0.31716   0.32115   0.32808
0.33073
 Alpha virt. eigenvalues --    0.33282   0.34392   0.34681   0.35000
0.35159
 Alpha virt. eigenvalues --    0.35411   0.35751   0.35869   0.35968
0.36598
 Alpha virt. eigenvalues --    0.37102   0.37491   0.38161   0.38756
0.39987
 Alpha virt. eigenvalues --    0.40497   0.40936   0.41829   0.42336
0.42682
 Alpha virt. eigenvalues --    0.43587   0.44125   0.44544   0.45630
0.46298
 Alpha virt. eigenvalues --    0.47353   0.48947   0.50492   0.51708
0.53460
 Alpha virt. eigenvalues --    0.56111   0.57224   0.57802   0.60026
0.61958
 Alpha virt. eigenvalues --    0.63523   0.65755   0.67377   0.68898
0.69054
 Alpha virt. eigenvalues --    0.70004   0.70574   0.71239   0.71582
0.72337
 Alpha virt. eigenvalues --    0.72910   0.73376   0.73979   0.74717
0.75278
 Alpha virt. eigenvalues --    0.75576   0.76048   0.76342   0.77192
0.77711
 Alpha virt. eigenvalues --    0.78463   0.79265   0.80248   0.81018
0.81693
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.81999   0.83056   0.83612   0.84272
0.85826
 Alpha virt. eigenvalues --    0.86705   0.87796   0.88831   0.89145
0.89929
 Alpha virt. eigenvalues --    0.90042   0.91533   0.92284   0.92501
0.92947
 Alpha virt. eigenvalues --    0.93390   0.94181   0.95299   0.95526
0.96438
 Alpha virt. eigenvalues --    0.97128   0.98194   1.00148   1.01148
1.02701
 Alpha virt. eigenvalues --    1.03210   1.03706   1.05153   1.06333
1.07844
 Alpha virt. eigenvalues --    1.08928   1.09904   1.10222   1.11533
1.13944
 Alpha virt. eigenvalues --    1.14334   1.14854   1.16453   1.17319
1.17782
 Alpha virt. eigenvalues --    1.18752   1.19412   1.20306   1.20820
1.22849
 Alpha virt. eigenvalues --    1.23997   1.24970   1.25722   1.26570
1.27076
 Alpha virt. eigenvalues --    1.28085   1.29113   1.30000   1.30261
1.31848
 Alpha virt. eigenvalues --    1.32023   1.33659   1.34753   1.35640
1.35909
 Alpha virt. eigenvalues --    1.36112   1.37216   1.38134   1.38703
1.39144
 Alpha virt. eigenvalues --    1.40300   1.42173   1.42479   1.42806
1.43684
 Alpha virt. eigenvalues --    1.43942   1.45226   1.45787   1.46188
1.47010
 Alpha virt. eigenvalues --    1.47506   1.48115   1.49293   1.50866
1.51220
 Alpha virt. eigenvalues --    1.52045   1.53693   1.54688   1.56512
1.57416
 Alpha virt. eigenvalues --    1.60059   1.63529   1.66023   1.66566
1.70181
 Alpha virt. eigenvalues --    1.72560   1.73610   1.74949   1.76371
1.77171
 Alpha virt. eigenvalues --    1.79047   1.79970   1.80533   1.81013
1.82974
 Alpha virt. eigenvalues --    1.83354   1.84312   1.84804   1.86289
1.87325
 Alpha virt. eigenvalues --    1.88274   1.88523   1.89607   1.90033
1.92143
 Alpha virt. eigenvalues --    1.92764   1.94197   1.94483   1.95405
1.96589
 Alpha virt. eigenvalues --    1.97147   1.97843   1.98451   1.99365
2.01189
 Alpha virt. eigenvalues --    2.03149   2.04212   2.06112   2.06351
2.08039
 Alpha virt. eigenvalues --    2.08819   2.10160   2.10763   2.12019
2.13103
```

```
 Alpha virt. eigenvalues --    2.15424   2.16691   2.17782   2.18826
2.19675
 Alpha virt. eigenvalues --    2.20409   2.23014   2.24881   2.25430
2.26374
 Alpha virt. eigenvalues --    2.27141   2.27907   2.28714   2.30594
2.31288
 Alpha virt. eigenvalues --    2.32146   2.33199   2.34517   2.37033
2.39477
 Alpha virt. eigenvalues --    2.40679   2.44147   2.44856   2.47949
2.49018
 Alpha virt. eigenvalues --    2.50536   2.54961   2.56857   2.58885
2.59651
 Alpha virt. eigenvalues --    2.61494   2.62308   2.62890   2.64410
2.65719
 Alpha virt. eigenvalues --    2.68112   2.69562   2.71078   2.71530
2.74494
 Alpha virt. eigenvalues --    2.74955   2.75081   2.79257   2.79849
2.81853
 Alpha virt. eigenvalues --    2.84383   2.85318   2.86126   2.87852
2.89840
 Alpha virt. eigenvalues --    2.92843   2.94760   2.96859   2.98877
3.09894
 Alpha virt. eigenvalues --    3.10933   3.15880   3.19009   3.22078
3.24232
 Alpha virt. eigenvalues --    3.24575   3.32748   3.41113   3.42271
4.24500
 Alpha virt. eigenvalues --    4.28483   4.29827   4.31802   4.32699
4.35224
 Alpha virt. eigenvalues --    4.36890   4.37971   4.38917   4.44904
4.47142
 Alpha virt. eigenvalues --    4.48349   4.49921   4.51416   4.54155
4.57238
 Alpha virt. eigenvalues --    4.60977   4.67917   4.70167   4.74328
4.83530
 Alpha virt. eigenvalues --    4.91917   5.25041
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   45.895413 -14.910790  16.662250 -13.212952   0.009501
0.709532
     2  C  -14.910790  33.519865 -15.709737  12.801827  -0.020610  -
0.887363
     3  C   16.662250 -15.709737  43.703726 -17.029931  -0.007287
0.418389
     4  C  -13.212952  12.801827 -17.029931  33.614195   0.251193  -
1.093320
     5  H    0.009501  -0.020610  -0.007287   0.251193   0.519788
0.001757
     6  C    0.709532  -0.887363   0.418389  -1.093320   0.001757
9.011155
     7  H    0.020336  -0.033750   0.037932  -0.099815  -0.002306
0.391845
```

This journal is © The Royal Society of Chemistry 2014

```
     8  C   -0.234055  -0.563522  -0.021228  -0.640165   0.016810  -
1.803346
     9  H    0.014609  -0.016430   0.011902  -0.019199  -0.000052  -
0.030900
    10  C  -19.786023   7.080583 -11.326451   6.482728  -0.002201  -
0.159210
    11  H   -0.105058  -0.046519   0.081365   0.020529   0.000002
0.000173
    12  C   -2.717565  -0.020857  -0.462196  -0.254440   0.003398  -
0.062142
    13  H    0.012794  -0.020182   0.034274   0.002000   0.000000
0.001827
    14  C   -0.475532   0.096486  -1.159512   0.535782   0.014953
0.054013
    15  H    0.042158   0.006415  -0.021737  -0.013692  -0.000007  -
0.001961
    16  C   -6.511569   3.329666 -15.737691   3.683847   0.033490
0.508552
    17  H    0.080393   0.016613  -0.038087  -0.032007   0.003951  -
0.014740
    18  C    2.990159 -12.923428   5.052212 -14.436016  -0.053606
0.268412
    19  C   -0.800047  -8.168936   0.601601  -9.084855   0.014366
0.103163
    20  C    0.132413   1.692467   0.444160   1.694278   0.008980  -
0.139417
    21  H   -0.017248  -0.005864  -0.004940   0.013605   0.000002  -
0.000916
    22  C    0.250222   0.588256  -0.003635   0.277595   0.002607  -
0.088938
    23  H   -0.003244  -0.020955   0.000368   0.001210   0.000000  -
0.000171
    24  C   -0.407246  -0.547409  -0.567676  -0.086712  -0.014473
0.040130
    25  H    0.000046   0.002294  -0.003275  -0.001808  -0.000008  -
0.000546
    26  C   -0.217365   1.555816   1.971810   0.972321   0.014898  -
0.117090
    27  H   -0.004434   0.017588  -0.023866  -0.009814   0.003728
0.001192
    28  C   -0.814705   1.211817  -0.752347   0.680820  -0.001962
0.806603
    29  C   -0.414203   0.588538  -0.187877   1.234977  -0.028002  -
1.465335
    30  O   -0.043412   0.034938  -0.091442   0.087017   0.000217  -
0.365870
    31  O    0.028898  -0.041878   0.170513  -0.137832   0.006157  -
0.084404
    32  O    0.224472  -0.127115   0.088949  -0.075662   0.000037  -
0.028361
    33  C   -0.075729  -2.365080   0.085046  -0.605636   0.002448
0.160686
```

34	H	-0.255035	-0.151679	-0.062658	0.011782	0.000000	0.008606
35	O	-0.131809	0.073621	-0.054143	0.036456	-0.000006	-0.002056

		7	8	9	10	11	12
1	C	0.020336	-0.234055	0.014609	-19.786023	-0.105058	-2.717565
2	C	-0.033750	-0.563522	-0.016430	7.080583	-0.046519	-0.020857
3	C	0.037932	-0.021228	0.011902	-11.326451	0.081365	-0.462196
4	C	-0.099815	-0.640165	-0.019199	6.482728	0.020529	-0.254440
5	H	-0.002306	0.016810	-0.000052	-0.002201	0.000002	0.003398
6	C	0.391845	-1.803346	-0.030900	-0.159210	0.000173	-0.062142
7	H	0.468040	-0.024331	-0.001973	0.000083	0.000000	0.001364
8	C	-0.024331	9.221731	0.377692	0.699080	-0.001770	0.229233
9	H	-0.001973	0.377692	0.450222	0.001359	-0.000001	0.000388
10	C	0.000083	0.699080	0.001359	23.064955	0.295234	-0.279612
11	H	0.000000	-0.001770	-0.000001	0.295234	0.534080	0.111173
12	C	0.001364	0.229233	0.000388	-0.279612	0.111173	9.938838
13	H	0.000000	-0.002129	0.000000	0.042524	-0.004622	0.256203
14	C	-0.001655	-0.009053	0.000064	-0.125200	0.018252	0.596344
15	H	0.000000	0.000897	0.000000	0.002921	-0.000165	-0.023277
16	C	0.013744	0.225399	-0.006606	7.300774	-0.031426	-0.100874
17	H	-0.000003	0.006799	0.000000	-0.021300	0.000017	-0.001792
18	C	0.128234	0.004933	0.012451	-2.983479	-0.012734	-0.249205
19	C	0.004720	-0.021768	0.020985	-2.161973	-0.046625	0.236740
20	C	-0.014895	-0.249176	-0.024754	-1.684966	0.003944	-0.303622
21	H	0.000000	0.002167	-0.000043	0.002843	-0.000001	0.000088
22	C	0.002296	0.046425	-0.007060	-0.040133	0.000201	0.046924
23	H	0.000000	0.000144	0.000000	0.000354	0.000000	0.000027

This journal is © The Royal Society of Chemistry 2014

24	C	-0.009389	-0.101996	-0.001070	0.024759	-0.000200	-0.018086
25	H	0.000002	0.000069	0.000000	-0.000087	0.000000	0.000003
26	C	-0.062839	-0.232206	-0.000404	-1.287462	0.000995	-0.285042
27	H	-0.000010	0.000482	0.000000	-0.000437	0.000000	-0.000228
28	C	0.018803	-1.915100	-0.084848	-0.036580	0.005816	-0.114371
29	C	-0.098469	0.813114	0.017437	0.118085	-0.000590	0.042996
30	O	0.007065	-0.202931	0.008421	0.007362	0.000079	0.002742
31	O	0.001772	-0.055266	-0.000553	-0.033218	0.000001	-0.001385
32	O	-0.000693	-0.094718	0.002879	-0.150403	-0.000382	-0.032260
33	C	-0.003470	0.412849	0.009982	0.948338	-0.014036	-0.156524
34	H	-0.000001	0.016970	0.000205	0.148271	0.002550	0.083215
35	O	-0.000028	-0.019073	0.000697	0.088483	0.001758	0.031572

		13	14	15	16	17	18
1	C	0.012794	-0.475532	0.042158	-6.511569	0.080393	2.990159
2	C	-0.020182	0.096486	0.006415	3.329666	0.016613	-12.923428
3	C	0.034274	-1.159512	-0.021737	-15.737691	-0.038087	5.052212
4	C	0.002000	0.535782	-0.013692	3.683847	-0.032007	-14.436016
5	H	0.000000	0.014953	-0.000007	0.033490	0.003951	-0.053606
6	C	0.001827	0.054013	-0.001961	0.508552	-0.014740	0.268412
7	H	0.000000	-0.001655	0.000000	0.013744	-0.000003	0.128234
8	C	-0.002129	-0.009053	0.000897	0.225399	0.006799	0.004933
9	H	0.000000	0.000064	0.000000	-0.006606	0.000000	0.012451
10	C	0.042524	-0.125200	0.002921	7.300774	-0.021300	-2.983479
11	H	-0.004622	0.018252	-0.000165	-0.031426	0.000017	-0.012734
12	C	0.256203	0.596344	-0.023277	-0.100874	-0.001792	-0.249205
13	H	0.519649	-0.046829	-0.004164	0.016604	-0.000160	0.003133

This journal is © The Royal Society of Chemistry 2014

14	C	-0.046829	7.646219	0.273467	0.089084	0.080717	-1.062394
15	H	-0.004164	0.273467	0.519168	0.030564	-0.004366	-0.002289
16	C	0.016604	0.089084	0.030564	17.640882	0.243586	-0.424803
17	H	-0.000160	0.080717	-0.004366	0.243586	0.525832	-0.055497
18	C	0.003133	-1.062394	-0.002289	-0.424803	-0.055497	39.255197
19	C	-0.001530	-0.542381	0.000769	-1.089003	-0.003247	11.200809
20	C	0.000057	0.088169	-0.000264	-1.036568	0.000772	-5.622458
21	H	0.000000	-0.000041	0.000000	0.000557	0.000000	0.040642
22	C	0.000009	0.001539	-0.000007	-0.102022	-0.000062	-0.560788
23	H	0.000000	-0.000008	0.000000	-0.000070	0.000000	0.036794
24	C	0.000012	-0.015706	0.000032	0.056100	-0.000440	1.013766
25	H	0.000000	0.000011	0.000000	0.000220	0.000000	-0.004665
26	C	-0.000084	0.136503	0.000175	-2.022161	0.004399	-13.768983
27	H	0.000000	0.000927	0.000000	0.004375	0.000003	-0.094808
28	C	0.002814	-0.068460	-0.001250	0.204025	-0.004225	0.267965
29	C	-0.001996	0.013284	0.003264	-0.427719	0.013941	-0.905316
30	O	-0.000017	0.027606	-0.000051	-0.030995	0.000348	-0.050772
31	O	0.000002	-0.028163	-0.000100	-0.087912	-0.000225	0.070041
32	O	-0.000071	0.000494	0.000004	-0.018524	0.000004	0.016449
33	C	-0.002286	0.139871	0.000339	0.322768	0.000301	-0.895016
34	H	-0.000006	0.003567	0.000000	0.005262	0.000000	-0.021892
35	O	-0.000003	-0.000094	0.000000	-0.000902	-0.000001	0.014383

		19	20	21	22	23	24
1	C	-0.800047	0.132413	-0.017248	0.250222	-0.003244	-0.407246
2	C	-8.168936	1.692467	-0.005864	0.588256	-0.020955	-0.547409
3	C	0.601601	0.444160	-0.004940	-0.003635	0.000368	-0.567676

This journal is © The Royal Society of Chemistry 2014

4	C	-9.084855	1.694278	0.013605	0.277595	0.001210	-0.086712
5	H	0.014366	0.008980	0.000002	0.002607	0.000000	-0.014473
6	C	0.103163	-0.139417	-0.000916	-0.088938	-0.000171	0.040130
7	H	0.004720	-0.014895	0.000000	0.002296	0.000000	-0.009389
8	C	-0.021768	-0.249176	0.002167	0.046425	0.000144	-0.101996
9	H	0.020985	-0.024754	-0.000043	-0.007060	0.000000	-0.001070
10	C	-2.161973	-1.684966	0.002843	-0.040133	0.000354	0.024759
11	H	-0.046625	0.003944	-0.000001	0.000201	0.000000	-0.000200
12	C	0.236740	-0.303622	0.000088	0.046924	0.000027	-0.018086
13	H	-0.001530	0.000057	0.000000	0.000009	0.000000	0.000012
14	C	-0.542381	0.088169	-0.000041	0.001539	-0.000008	-0.015706
15	H	0.000769	-0.000264	0.000000	-0.000007	0.000000	0.000032
16	C	-1.089003	-1.036568	0.000557	-0.102022	-0.000070	0.056100
17	H	-0.003247	0.000772	0.000000	-0.000062	0.000000	-0.000440
18	C	11.200809	-5.622458	0.040642	-0.560788	0.036794	1.013766
19	C	31.001156	-9.084449	-0.150743	-2.073202	0.016535	0.976074
20	C	-9.084449	14.653089	0.345928	0.339569	0.038744	-0.699984
21	H	-0.150743	0.345928	0.472417	0.087352	-0.004178	0.010864
22	C	-2.073202	0.339569	0.087352	7.315307	0.270992	0.140304
23	H	0.016535	0.038744	-0.004178	0.270992	0.519735	-0.029076
24	C	0.976074	-0.699984	0.010864	0.140304	-0.029076	7.269831
25	H	0.017819	0.010091	-0.000147	-0.030160	-0.004036	0.296226
26	C	-4.454865	6.035571	-0.008230	0.019562	-0.013394	-1.143756
27	H	0.075943	-0.023603	0.000015	0.001008	-0.000158	0.027332
28	C	0.223156	0.124913	0.000316	0.001788	0.000092	0.024295
29	C	-0.314624	0.005773	-0.000198	0.023007	-0.000079	0.052308

This journal is © The Royal Society of Chemistry 2014

30	O	0.002575	0.022990	0.000001	0.000201	0.000000	0.000137
31	O	0.021027	0.004160	0.000000	0.000332	0.000000	-0.002072
32	O	0.001658	0.003542	0.000003	-0.001359	0.000000	-0.000358
33	C	-0.434197	-0.615729	-0.022365	-0.227861	-0.001393	-0.064219
34	H	0.071438	-0.017200	-0.000072	0.004896	0.000000	-0.000362
35	O	-0.037960	-0.088958	-0.005141	0.086156	0.000179	-0.001611

		25	26	27	28	29	30
1	C	0.000046	-0.217365	-0.004434	-0.814705	-0.414203	-0.043412
2	C	0.002294	1.555816	0.017588	1.211817	0.588538	0.034938
3	C	-0.003275	1.971810	-0.023866	-0.752347	-0.187877	-0.091442
4	C	-0.001808	0.972321	-0.009814	0.680820	1.234977	0.087017
5	H	-0.000008	0.014898	0.003728	-0.001962	-0.028002	0.000217
6	C	-0.000546	-0.117090	0.001192	0.806603	-1.465335	-0.365870
7	H	0.000002	-0.062839	-0.000010	0.018803	-0.098469	0.007065
8	C	0.000069	-0.232206	0.000482	-1.915100	0.813114	-0.202931
9	H	0.000000	-0.000404	0.000000	-0.084848	0.017437	0.008421
10	C	-0.000087	-1.287462	-0.000437	-0.036580	0.118085	0.007362
11	H	0.000000	0.000995	0.000000	0.005816	-0.000590	0.000079
12	C	0.000003	-0.285042	-0.000228	-0.114371	0.042996	0.002742
13	H	0.000000	-0.000084	0.000000	0.002814	-0.001996	-0.000017
14	C	0.000011	0.136503	0.000927	-0.068460	0.013284	0.027606
15	H	0.000000	0.000175	0.000000	-0.001250	0.003264	-0.000051
16	C	0.000220	-2.022161	0.004375	0.204025	-0.427719	-0.030995
17	H	0.000000	0.004399	0.000003	-0.004225	0.013941	0.000348
18	C	-0.004665	-13.768983	-0.094808	0.267965	-0.905316	-0.050772
19	C	0.017819	-4.454865	0.075943	0.223156	-0.314624	0.002575

This journal is © The Royal Society of Chemistry 2014

20	C	0.010091	6.035571	-0.023603	0.124913	0.005773
0.022990						
21	H	-0.000147	-0.008230	0.000015	0.000316	-0.000198
0.000001						
22	C	-0.030160	0.019562	0.001008	0.001788	0.023007
0.000201						
23	H	-0.004036	-0.013394	-0.000158	0.000092	-0.000079
0.000000						
24	C	0.296226	-1.143756	0.027332	0.024295	0.052308
0.000137						
25	H	0.521150	0.010191	-0.004329	-0.000036	0.000082
0.000000						
26	C	0.010191	18.474500	0.305017	-0.023117	0.144590
0.024751						
27	H	-0.004329	0.305017	0.532635	-0.001106	0.004384
0.000005						
28	C	-0.000036	-0.023117	-0.001106	7.131749	-1.043514
0.238888						
29	C	0.000082	0.144590	0.004384	-1.043514	6.794727
0.322020						
30	O	0.000000	0.024751	0.000005	0.238888	0.322020
8.318712						
31	O	0.000000	0.018517	-0.000004	0.039463	0.439492	-
0.087202						
32	O	0.000000	0.004111	0.000000	0.432559	0.017820	-
0.068981						
33	C	0.000204	-0.082123	0.000662	-0.641413	0.019765
0.029831						
34	H	0.000000	-0.006220	0.000000	-0.007626	0.000418	-
0.000289						
35	O	0.000010	-0.039134	-0.000005	0.003556	-0.000629	-
0.000198						

		31	32	33	34	35
1	C	0.028898	0.224472	-0.075729	-0.255035	-0.131809
2	C	-0.041878	-0.127115	-2.365080	-0.151679	0.073621
3	C	0.170513	0.088949	0.085046	-0.062658	-0.054143
4	C	-0.137832	-0.075662	-0.605636	0.011782	0.036456
5	H	0.006157	0.000037	0.002448	0.000000	-0.000006
6	C	-0.084404	-0.028361	0.160686	0.008606	-0.002056
7	H	0.001772	-0.000693	-0.003470	-0.000001	-0.000028
8	C	-0.055266	-0.094718	0.412849	0.016970	-0.019073
9	H	-0.000553	0.002879	0.009982	0.000205	0.000697
10	C	-0.033218	-0.150403	0.948338	0.148271	0.088483
11	H	0.000001	-0.000382	-0.014036	0.002550	0.001758
12	C	-0.001385	-0.032260	-0.156524	0.083215	0.031572
13	H	0.000002	-0.000071	-0.002286	-0.000006	-0.000003
14	C	-0.028163	0.000494	0.139871	0.003567	-0.000094
15	H	-0.000100	0.000004	0.000339	0.000000	0.000000
16	C	-0.087912	-0.018524	0.322768	0.005262	-0.000902
17	H	-0.000225	0.000004	0.000301	0.000000	-0.000001
18	C	0.070041	0.016449	-0.895016	-0.021892	0.014383
19	C	0.021027	0.001658	-0.434197	0.071438	-0.037960

This journal is © The Royal Society of Chemistry 2014

20	C	0.004160	0.003542	-0.615729	-0.017200	-0.088958
21	H	0.000000	0.000003	-0.022365	-0.000072	-0.005141
22	C	0.000332	-0.001359	-0.227861	0.004896	0.086156
23	H	0.000000	0.000000	-0.001393	0.000000	0.000179
24	C	-0.002072	-0.000358	-0.064219	-0.000362	-0.001611
25	H	0.000000	0.000000	0.000204	0.000000	0.000010
26	C	0.018517	0.004111	-0.082123	-0.006220	-0.039134
27	H	-0.000004	0.000000	0.000662	0.000000	-0.000005
28	C	0.039463	0.432559	-0.641413	-0.007626	0.003556
29	C	0.439492	0.017820	0.019765	0.000418	-0.000629
30	O	-0.087202	-0.068981	0.029831	-0.000289	-0.000198
31	O	8.140364	0.000241	0.003005	0.000008	0.000003
32	O	0.000241	8.134062	0.046249	-0.003173	-0.000514
33	C	0.003005	0.046249	9.135632	0.416510	0.364506
34	H	0.000008	-0.003173	0.416510	0.590046	-0.030766
35	O	0.000003	-0.000514	0.364506	-0.030766	8.020687

Mulliken atomic charges:

		1
1	C	0.064825
2	C	-0.034684
3	C	-0.098783
4	C	0.431692
5	H	0.222238
6	C	-0.139949
7	H	0.257389
8	C	0.117037
9	H	0.264600
10	C	-0.230002
11	H	0.187961
12	C	-0.497770
13	H	0.192179
14	C	-0.282325
15	H	0.193157
16	C	-0.080652
17	H	0.198476
18	C	-0.247431
19	C	-0.120129
20	C	-0.043566
21	H	0.243326
22	C	-0.371323
23	H	0.191586
24	C	-0.220332
25	H	0.190680
26	C	0.070747
27	H	0.187506
28	C	0.091220
29	C	0.218527
30	O	-0.193745
31	O	-0.383781
32	O	-0.370960
33	C	0.108085
34	H	0.193236

This journal is © The Royal Society of Chemistry 2014

```
   35  O   -0.309036
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  C    0.064825
    2  C   -0.034684
    3  C   -0.098783
    4  C    0.653930
    5  H    0.000000
    6  C    0.117441
    7  H    0.000000
    8  C    0.381637
    9  H    0.000000
   10  C   -0.042041
   11  H    0.000000
   12  C   -0.305591
   13  H    0.000000
   14  C   -0.089168
   15  H    0.000000
   16  C    0.117824
   17  H    0.000000
   18  C   -0.247431
   19  C   -0.120129
   20  C    0.199760
   21  H    0.000000
   22  C   -0.179736
   23  H    0.000000
   24  C   -0.029652
   25  H    0.000000
   26  C    0.258253
   27  H    0.000000
   28  C    0.091220
   29  C    0.218527
   30  O   -0.193745
   31  O   -0.383781
   32  O   -0.370960
   33  C    0.301321
   34  H    0.000000
   35  O   -0.309036
Sum of Mulliken charges=   0.00000
Electronic spatial extent (au):  <R**2>=  5389.5964
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     3.2626    Y=    -2.6385    Z=     3.2668  Tot=     5.3178
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=  -132.2533   YY=  -139.2020   ZZ=  -132.9626
  XY=   -11.2796   XZ=   -14.0927   YZ=     4.7019
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=     2.5526   YY=    -4.3960   ZZ=     1.8434
  XY=   -11.2796   XZ=   -14.0927   YZ=     4.7019
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=    53.2175  YYY=   -23.4302  ZZZ=   -26.6990  XYY=     5.1143
```

This journal is © The Royal Society of Chemistry 2014


```
  XXY=    -5.7879  XXZ=    40.1971  XZZ=   -18.4340  YZZ=    -4.3208
  YYZ=    35.4181  XYZ=     2.0582
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX= -3447.2900 YYYY= -2072.1139 ZZZZ= -1654.5996 XXXY=   -55.9929
 XXXZ=  -109.7645 YYYX=  -139.4891 YYYZ=    19.6305 ZZZX=   -39.7777
 ZZZY=    25.1164 XXYY=  -991.1802 XXZZ=  -897.4767 YYZZ=  -625.9842
 XXYZ=    -0.3069 YYXZ=   -47.0393 ZZXY=    22.5555
 N-N= 1.906954456088D+03 E-N=-6.213457845153D+03  KE=
1.022584807371D+03
 1\1\GINC-OPT0790\FTS\RB3LYP\6-31+G(d)\C19H12O4\UCN0868\04-Nov-
2011\0\\
 # opt=(calcfc,ts) b3lyp/6-31+g(d) geom=connectivity\\Title Card
Requir
 ed\\0,1\C,-
0.5561133767,0.5228024908,1.1630684408\C,0.6042357606,1.084
 8772875,0.4911365185\C,-0.7415902387,-
0.8839315711,1.0599307682\C,0.22
 575928,-1.6046861347,0.264954633\H,0.0634054087,-
2.6745493089,0.144276
 5616\C,-0.2033072393,-0.9632987852,-1.6362732815\H,0.4927341692,-
1.645
 3952033,-2.1105092922\C,-0.0960823924,0.4431716352,-
1.7195032737\H,0.7
 376080326,1.0037227105,-2.1188115584\C,-
1.5159563395,1.2809880262,1.87
 77554081\H,-1.3928857678,2.3517011966,1.9995892586\C,-
2.6012920712,0.6
 550530981,2.4691103466\H,-3.3165751025,1.2459736088,3.0345026842\C,-
2.
 7868778083,-0.7363407253,2.3460831432\H,-3.6475607125,-
1.2109357728,2.
 808726619\C,-1.8740162769,-1.4967510814,1.6348320879\H,-
2.0129950485,-
 2.5688529751,1.5241409233\C,1.597329566,-
1.1435548856,0.3198534284\C,1

.8022660823,0.2618824521,0.4112505163\C,3.128141571,0.7578080062,0.359
 8060915\H,3.2998345613,1.8241663682,0.4156090031\C,4.1960640524,-
0.121

3179032,0.254537311\H,5.2096696188,0.2705812249,0.246405438\C,3.985046
 5086,-1.5105759827,0.1573690277\H,4.8330221088,-
2.1849653208,0.0732945
 061\C,2.6942513389,-2.0151474193,0.171099071\H,2.5177909424,-
3.0853638
 052,0.0902115012\C,-1.4618978756,0.9927300797,-1.7825363829\C,-
1.66102
 0977,-1.2774356785,-1.7342003892\O,-2.3652658583,-0.082413086,-
1.69317
 71414\O,-2.211104345,-2.3440014829,-1.8122402207\O,-
1.8548586483,2.125
```

This journal is © The Royal Society of Chemistry 2014

0070125,-1.8912623551\C,0.6285683745,2.5565953961,0.2500928211\H,-
0.36

28381767,3.0405447586,0.2551805388\O,1.6229758791,3.2188437702,0.00056
82476\\Version=AM64L-G03RevD.01\State=1-A\HF=-
1032.138019\RMSD=7.313e-
09\RMSF=1.547e-06\Thermal=0.\Dipole=1.2668075,-
1.2017982,1.1524258\PG=
C01 [X(C19H12O4)]\\@

KINETICS FACT
--- = ---
MECHANISM FICTION
Job cpu time: 1 days 16 hours 59 minutes 26.1 seconds.
File lengths (MBytes): RWF= 591 Int= 0 D2E= 0 Chk=
20 Scr= 1
Normal termination of Gaussian 03 at Fri Nov 4 23:20:20 2011.

This journal is © The Royal Society of Chemistry 2014

(15S)-12,14-dioxo-9,10,11,12,14,15-hexahydro-9,10-[3,4]furanoanthracene-9-carbaldehyde

```
Entering Link 1 = C:\G09W\l1.exe PID=      8624.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2009, Gaussian, Inc.
                    All Rights Reserved.

 This is part of the Gaussian(R) 09 program.  It is based on
 the Gaussian(R) 03 system (copyright 2003, Gaussian, Inc.),
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,
 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be
 used, copied, transmitted, or stored only in accord with that
 written license.

 The following legend is applicable only to US Government
 contracts under FAR:

                       RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is
 subject to restrictions as set forth in subparagraphs (a)
 and (c) of the Commercial Computer Software - Restricted
 Rights clause in FAR 52.227-19.

 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ----------------------------------------------------------------
 Warning -- This program may not be used in any manner that
 competes with the business of Gaussian, Inc. or will provide
 assistance to any competitor of Gaussian, Inc.  The licensee
 of this program is prohibited from giving any competitor of
 Gaussian, Inc. access to this program.  By using this program,
 the user acknowledges that Gaussian, Inc. is engaged in the
```

This journal is © The Royal Society of Chemistry 2014

```
 business of creating and licensing software in the field of
 computational chemistry and represents and warrants to the
 licensee that it is not a competitor of Gaussian, Inc. and that
 it will not use this program in any manner prohibited above.
 ----------------------------------------------------------------


 Cite this work as:
 Gaussian 09, Revision A.02,
 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
 M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
 G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
 A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
 M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
 Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
 J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
 K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand,
 K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
 M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
 V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
 O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
 R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
 P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
 O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
 and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

 ******************************************
 Gaussian 09:  IA32W-G09RevA.02 11-Jun-2009
               24-Jul-2013
 ******************************************
 %mem=64MW
 %chk=F:\solid state\Mack group papers\Ball mill energetics\James
Calculations\Al
 dehydeAnthraceneCalculations\9FORMYLANTHRACENEPRODUCT2.chk
 ---------------------------------------
 # opt b3lyp/6-31+g(d) geom=connectivity
 ---------------------------------------
 1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
 2/9=110,12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
 4//1;
 5/5=2,38=5/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 7//1,2,3,16;
 1/14=-1,18=20,19=15/3(2);
 2/9=110/2;
 99//99;
 2/9=110/2;
 3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
 4/5=5,16=3/1;
 5/5=2,38=5/2;
 7//1,2,3,16;
```

This journal is © The Royal Society of Chemistry 2014

```
 1/14=-1,18=20,19=15/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 ----------------------------
 9-formylanthracene DA product
 ----------------------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                    -1.62501  -1.03639  -0.39027
 C                    -0.18984  -1.43829  -0.66535
 H                    -0.09685  -2.4456   -1.07791
 C                    -1.75248   0.26007   0.13746
 C                     0.33566  -0.37569  -1.6973
 H                    -0.24609  -0.46263  -2.61928
 C                     0.59459  -1.2589    0.62174
 C                     0.47831   0.02539   1.18683
 C                    -0.39605   0.96564   0.35122
 C                     0.27263   1.0292   -1.07137
 H                    -0.27568   1.75702  -1.6758
 C                     1.39002  -2.22765   1.22671
 H                     1.48167  -3.21397   0.77917
 C                     1.18041   0.3355    2.35104
 H                     1.13745   1.32898   2.78595
 C                     1.96821  -0.64535   2.9638
 H                     2.50937  -0.40381   3.87417
 C                     2.07155  -1.92008   2.40834
 H                     2.68976  -2.67384   2.88756
 C                    -2.75474  -1.80602  -0.64798
 H                    -2.64986  -2.80649  -1.06077
 C                    -4.02261  -1.28355  -0.37056
 H                    -4.90784  -1.88335  -0.56261
 C                    -4.15083   0.00612   0.14361
 H                    -5.13647   0.41367   0.34974
 C                    -3.01639   0.78741   0.39327
 H                    -3.13323   1.79789   0.77234
 C                     1.80403  -0.57881  -2.03679
 C                     1.73268   1.46722  -0.99522
 O                     2.54025   0.51997  -1.6167
 O                     2.19752   2.44736  -0.49102
 O                     2.32097  -1.51826  -2.56948
 C                    -0.61348   2.36006   0.92458
 H                    -0.58327   2.44124   2.03016
 O                    -0.88736   3.32039   0.24154


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Initialization pass.
                          ----------------------------
```

This journal is © The Royal Society of Chemistry 2014

! Initial Parameters !
! (Angstroms and Degrees) !

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.5156	estimate D2E/DX2
R2	R(1,4)	1.4055	estimate D2E/DX2
R3	R(1,20)	1.3911	estimate D2E/DX2
R4	R(2,3)	1.0925	estimate D2E/DX2
R5	R(2,5)	1.5717	estimate D2E/DX2
R6	R(2,7)	1.5179	estimate D2E/DX2
R7	R(4,9)	1.5438	estimate D2E/DX2
R8	R(4,26)	1.3932	estimate D2E/DX2
R9	R(5,6)	1.0936	estimate D2E/DX2
R10	R(5,10)	1.5393	estimate D2E/DX2
R11	R(5,28)	1.5207	estimate D2E/DX2
R12	R(7,8)	1.4079	estimate D2E/DX2
R13	R(7,12)	1.3918	estimate D2E/DX2
R14	R(8,9)	1.5319	estimate D2E/DX2
R15	R(8,14)	1.3945	estimate D2E/DX2
R16	R(9,10)	1.5732	estimate D2E/DX2
R17	R(9,33)	1.5233	estimate D2E/DX2
R18	R(10,11)	1.0935	estimate D2E/DX2
R19	R(10,29)	1.5262	estimate D2E/DX2
R20	R(12,13)	1.087	estimate D2E/DX2
R21	R(12,18)	1.3983	estimate D2E/DX2
R22	R(14,15)	1.0854	estimate D2E/DX2

This journal is © The Royal Society of Chemistry 2014

```
 ! R23   R(14,16)              1.3993         estimate D2E/DX2
!
 ! R24   R(16,17)              1.0863         estimate D2E/DX2
!
 ! R25   R(16,18)              1.3943         estimate D2E/DX2
!
 ! R26   R(18,19)              1.0863         estimate D2E/DX2
!
 ! R27   R(20,21)              1.0874         estimate D2E/DX2
!
 ! R28   R(20,22)              1.3991         estimate D2E/DX2
!
 ! R29   R(22,23)              1.0864         estimate D2E/DX2
!
 ! R30   R(22,24)              1.3943         estimate D2E/DX2
!
 ! R31   R(24,25)              1.0863         estimate D2E/DX2
!
 ! R32   R(24,26)              1.3999         estimate D2E/DX2
!
 ! R33   R(26,27)              1.0855         estimate D2E/DX2
!
 ! R34   R(28,30)              1.3877         estimate D2E/DX2
!
 ! R35   R(28,32)              1.1973         estimate D2E/DX2
!
 ! R36   R(29,30)              1.3913         estimate D2E/DX2
!
 ! R37   R(29,31)              1.1962         estimate D2E/DX2
!
 ! R38   R(33,34)              1.109          estimate D2E/DX2
!
 ! R39   R(33,35)              1.2099         estimate D2E/DX2
!
 ! A1    A(2,1,4)            113.4927         estimate D2E/DX2
!
 ! A2    A(2,1,20)           126.066          estimate D2E/DX2
!
 ! A3    A(4,1,20)           120.4135         estimate D2E/DX2
!
 ! A4    A(1,2,3)            113.1817         estimate D2E/DX2
!
 ! A5    A(1,2,5)            104.8629         estimate D2E/DX2
!
 ! A6    A(1,2,7)            107.7053         estimate D2E/DX2
!
 ! A7    A(3,2,5)            110.3025         estimate D2E/DX2
!
 ! A8    A(3,2,7)            112.6553         estimate D2E/DX2
!
 ! A9    A(5,2,7)            107.701          estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A10   A(1,4,9)              113.195          estimate D2E/DX2
!
 ! A11   A(1,4,26)             120.0233         estimate D2E/DX2
!
 ! A12   A(9,4,26)             126.7741         estimate D2E/DX2
!
 ! A13   A(2,5,6)              108.7795         estimate D2E/DX2
!
 ! A14   A(2,5,10)             109.6564         estimate D2E/DX2
!
 ! A15   A(2,5,28)             112.2787         estimate D2E/DX2
!
 ! A16   A(6,5,10)             113.1777         estimate D2E/DX2
!
 ! A17   A(6,5,28)             108.3487         estimate D2E/DX2
!
 ! A18   A(10,5,28)            104.6086         estimate D2E/DX2
!
 ! A19   A(2,7,8)              113.919          estimate D2E/DX2
!
 ! A20   A(2,7,12)             125.566          estimate D2E/DX2
!
 ! A21   A(8,7,12)             120.5078         estimate D2E/DX2
!
 ! A22   A(7,8,9)              112.8355         estimate D2E/DX2
!
 ! A23   A(7,8,14)             119.7602         estimate D2E/DX2
!
 ! A24   A(9,8,14)             127.3202         estimate D2E/DX2
!
 ! A25   A(4,9,8)              107.2468         estimate D2E/DX2
!
 ! A26   A(4,9,10)             105.4686         estimate D2E/DX2
!
 ! A27   A(4,9,33)             110.1859         estimate D2E/DX2
!
 ! A28   A(8,9,10)             105.988          estimate D2E/DX2
!
 ! A29   A(8,9,33)             115.9767         estimate D2E/DX2
!
 ! A30   A(10,9,33)            111.349          estimate D2E/DX2
!
 ! A31   A(5,10,9)             110.3791         estimate D2E/DX2
!
 ! A32   A(5,10,11)            113.7808         estimate D2E/DX2
!
 ! A33   A(5,10,29)            104.0668         estimate D2E/DX2
!
 ! A34   A(9,10,11)            108.2761         estimate D2E/DX2
!
 ! A35   A(9,10,29)            111.9065         estimate D2E/DX2
!
```

```
 ! A36   A(11,10,29)           108.4362         estimate D2E/DX2
!
 ! A37   A(7,12,13)            120.053          estimate D2E/DX2
!
 ! A38   A(7,12,18)            119.5215         estimate D2E/DX2
!
 ! A39   A(13,12,18)           120.4251         estimate D2E/DX2
!
 ! A40   A(8,14,15)            121.2105         estimate D2E/DX2
!
 ! A41   A(8,14,16)            119.5485         estimate D2E/DX2
!
 ! A42   A(15,14,16)           119.2368         estimate D2E/DX2
!
 ! A43   A(14,16,17)           119.4454         estimate D2E/DX2
!
 ! A44   A(14,16,18)           120.5372         estimate D2E/DX2
!
 ! A45   A(17,16,18)           120.0146         estimate D2E/DX2
!
 ! A46   A(12,18,16)           120.1055         estimate D2E/DX2
!
 ! A47   A(12,18,19)           119.8381         estimate D2E/DX2
!
 ! A48   A(16,18,19)           120.0537         estimate D2E/DX2
!
 ! A49   A(1,20,21)            120.0702         estimate D2E/DX2
!
 ! A50   A(1,20,22)            119.5132         estimate D2E/DX2
!
 ! A51   A(21,20,22)           120.4166         estimate D2E/DX2
!
 ! A52   A(20,22,23)           119.8137         estimate D2E/DX2
!
 ! A53   A(20,22,24)           120.1243         estimate D2E/DX2
!
 ! A54   A(23,22,24)           120.061          estimate D2E/DX2
!
 ! A55   A(22,24,25)           120.0288         estimate D2E/DX2
!
 ! A56   A(22,24,26)           120.4953         estimate D2E/DX2
!
 ! A57   A(25,24,26)           119.4754         estimate D2E/DX2
!
 ! A58   A(4,26,24)            119.4181         estimate D2E/DX2
!
 ! A59   A(4,26,27)            120.9378         estimate D2E/DX2
!
 ! A60   A(24,26,27)           119.6406         estimate D2E/DX2
!
 ! A61   A(5,28,30)            109.8111         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A62   A(5,28,32)            128.3901         estimate D2E/DX2
!
 ! A63   A(30,28,32)           121.7947         estimate D2E/DX2
!
 ! A64   A(10,29,30)           109.7302         estimate D2E/DX2
!
 ! A65   A(10,29,31)           128.8967         estimate D2E/DX2
!
 ! A66   A(30,29,31)           121.3705         estimate D2E/DX2
!
 ! A67   A(28,30,29)           111.4909         estimate D2E/DX2
!
 ! A68   A(9,33,34)            115.9997         estimate D2E/DX2
!
 ! A69   A(9,33,35)            123.1212         estimate D2E/DX2
!
 ! A70   A(34,33,35)           120.7231         estimate D2E/DX2
!
 ! D1    D(4,1,2,3)           -179.8405         estimate D2E/DX2
!
 ! D2    D(4,1,2,5)            -59.5648         estimate D2E/DX2
!
 ! D3    D(4,1,2,7)             54.9507         estimate D2E/DX2
!
 ! D4    D(20,1,2,3)            -1.7631         estimate D2E/DX2
!
 ! D5    D(20,1,2,5)           118.5126         estimate D2E/DX2
!
 ! D6    D(20,1,2,7)          -126.9719         estimate D2E/DX2
!
 ! D7    D(2,1,4,9)             -1.5133         estimate D2E/DX2
!
 ! D8    D(2,1,4,26)           177.55           estimate D2E/DX2
!
 ! D9    D(20,1,4,9)          -179.7113         estimate D2E/DX2
!
 ! D10   D(20,1,4,26)           -0.648          estimate D2E/DX2
!
 ! D11   D(2,1,20,21)            1.7478         estimate D2E/DX2
!
 ! D12   D(2,1,20,22)         -178.3332         estimate D2E/DX2
!
 ! D13   D(4,1,20,21)          179.7032         estimate D2E/DX2
!
 ! D14   D(4,1,20,22)           -0.3778         estimate D2E/DX2
!
 ! D15   D(1,2,5,6)            -63.2278         estimate D2E/DX2
!
 ! D16   D(1,2,5,10)            61.0285         estimate D2E/DX2
!
 ! D17   D(1,2,5,28)           176.8627         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D18   D(3,2,5,6)             58.9424         estimate D2E/DX2
!
 ! D19   D(3,2,5,10)          -176.8013         estimate D2E/DX2
!
 ! D20   D(3,2,5,28)           -60.9671         estimate D2E/DX2
!
 ! D21   D(7,2,5,6)           -177.7462         estimate D2E/DX2
!
 ! D22   D(7,2,5,10)           -53.4899         estimate D2E/DX2
!
 ! D23   D(7,2,5,28)            62.3442         estimate D2E/DX2
!
 ! D24   D(1,2,7,8)            -53.6408         estimate D2E/DX2
!
 ! D25   D(1,2,7,12)           127.3363         estimate D2E/DX2
!
 ! D26   D(3,2,7,8)           -179.1632         estimate D2E/DX2
!
 ! D27   D(3,2,7,12)             1.8139         estimate D2E/DX2
!
 ! D28   D(5,2,7,8)             58.9739         estimate D2E/DX2
!
 ! D29   D(5,2,7,12)          -120.049          estimate D2E/DX2
!
 ! D30   D(1,4,9,8)             -52.8708         estimate D2E/DX2
!
 ! D31   D(1,4,9,10)            59.7826         estimate D2E/DX2
!
 ! D32   D(1,4,9,33)          -179.9397         estimate D2E/DX2
!
 ! D33   D(26,4,9,8)           128.1418         estimate D2E/DX2
!
 ! D34   D(26,4,9,10)         -119.2048         estimate D2E/DX2
!
 ! D35   D(26,4,9,33)            1.0728         estimate D2E/DX2
!
 ! D36   D(1,4,26,24)            1.1864         estimate D2E/DX2
!
 ! D37   D(1,4,26,27)         -178.1272         estimate D2E/DX2
!
 ! D38   D(9,4,26,24)         -179.8886         estimate D2E/DX2
!
 ! D39   D(9,4,26,27)            0.7979         estimate D2E/DX2
!
 ! D40   D(2,5,10,9)            -4.2997         estimate D2E/DX2
!
 ! D41   D(2,5,10,11)         -126.2557         estimate D2E/DX2
!
 ! D42   D(2,5,10,29)          115.9248         estimate D2E/DX2
!
 ! D43   D(6,5,10,9)           117.3545         estimate D2E/DX2
!
```

```
 ! D44   D(6,5,10,11)           -4.6016         estimate D2E/DX2
!
 ! D45   D(6,5,10,29)         -122.421          estimate D2E/DX2
!
 ! D46   D(28,5,10,9)         -124.9049         estimate D2E/DX2
!
 ! D47   D(28,5,10,11)         113.139          estimate D2E/DX2
!
 ! D48   D(28,5,10,29)          -4.6804         estimate D2E/DX2
!
 ! D49   D(2,5,28,30)         -116.2796         estimate D2E/DX2
!
 ! D50   D(2,5,28,32)           62.9853         estimate D2E/DX2
!
 ! D51   D(6,5,28,30)          123.5606         estimate D2E/DX2
!
 ! D52   D(6,5,28,32)          -57.1745         estimate D2E/DX2
!
 ! D53   D(10,5,28,30)           2.5656         estimate D2E/DX2
!
 ! D54   D(10,5,28,32)        -178.1696         estimate D2E/DX2
!
 ! D55   D(2,7,8,9)             -1.2481         estimate D2E/DX2
!
 ! D56   D(2,7,8,14)          -178.1553         estimate D2E/DX2
!
 ! D57   D(12,7,8,9)           177.8294         estimate D2E/DX2
!
 ! D58   D(12,7,8,14)            0.9222         estimate D2E/DX2
!
 ! D59   D(2,7,12,13)           -0.4802         estimate D2E/DX2
!
 ! D60   D(2,7,12,18)          179.2843         estimate D2E/DX2
!
 ! D61   D(8,7,12,13)         -179.4435         estimate D2E/DX2
!
 ! D62   D(8,7,12,18)            0.321          estimate D2E/DX2
!
 ! D63   D(7,8,9,4)             54.1924         estimate D2E/DX2
!
 ! D64   D(7,8,9,10)           -58.1074         estimate D2E/DX2
!
 ! D65   D(7,8,9,33)           177.7776         estimate D2E/DX2
!
 ! D66   D(14,8,9,4)          -129.184          estimate D2E/DX2
!
 ! D67   D(14,8,9,10)          118.5161         estimate D2E/DX2
!
 ! D68   D(14,8,9,33)           -5.5988         estimate D2E/DX2
!
 ! D69   D(7,8,14,15)          177.6777         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D70   D(7,8,14,16)           -1.5665         estimate D2E/DX2
!
 ! D71   D(9,8,14,15)            1.2626         estimate D2E/DX2
!
 ! D72   D(9,8,14,16)         -177.9817         estimate D2E/DX2
!
 ! D73   D(4,9,10,5)           -54.0558         estimate D2E/DX2
!
 ! D74   D(4,9,10,11)           71.0927         estimate D2E/DX2
!
 ! D75   D(4,9,10,29)         -169.4501         estimate D2E/DX2
!
 ! D76   D(8,9,10,5)            59.4785         estimate D2E/DX2
!
 ! D77   D(8,9,10,11)         -175.3729         estimate D2E/DX2
!
 ! D78   D(8,9,10,29)          -55.9157         estimate D2E/DX2
!
 ! D79   D(33,9,10,5)         -173.5663         estimate D2E/DX2
!
 ! D80   D(33,9,10,11)         -48.4178         estimate D2E/DX2
!
 ! D81   D(33,9,10,29)          71.0394         estimate D2E/DX2
!
 ! D82   D(4,9,33,34)           93.001          estimate D2E/DX2
!
 ! D83   D(4,9,33,35)          -82.4823         estimate D2E/DX2
!
 ! D84   D(8,9,33,34)          -29.0396         estimate D2E/DX2
!
 ! D85   D(8,9,33,35)          155.4771         estimate D2E/DX2
!
 ! D86   D(10,9,33,34)        -150.332          estimate D2E/DX2
!
 ! D87   D(10,9,33,35)          34.1846         estimate D2E/DX2
!
 ! D88   D(5,10,29,30)           5.5126         estimate D2E/DX2
!
 ! D89   D(5,10,29,31)        -173.9007         estimate D2E/DX2
!
 ! D90   D(9,10,29,30)         124.7018         estimate D2E/DX2
!
 ! D91   D(9,10,29,31)          -54.7116         estimate D2E/DX2
!
 ! D92   D(11,10,29,30)       -115.9352         estimate D2E/DX2
!
 ! D93   D(11,10,29,31)         64.6515         estimate D2E/DX2
!
 ! D94   D(7,12,18,16)          -0.9087         estimate D2E/DX2
!
 ! D95   D(7,12,18,19)         179.6903         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D96   D(13,12,18,16)        178.8549         estimate D2E/DX2
!
 ! D97   D(13,12,18,19)         -0.546          estimate D2E/DX2
!
 ! D98   D(8,14,16,17)        -179.6099         estimate D2E/DX2
!
 ! D99   D(8,14,16,18)           0.9881         estimate D2E/DX2
!
 ! D100  D(15,14,16,17)          1.1309         estimate D2E/DX2
!
 ! D101  D(15,14,16,18)       -178.2712         estimate D2E/DX2
!
 ! D102  D(14,16,18,12)          0.2572         estimate D2E/DX2
!
 ! D103  D(14,16,18,19)        179.6569         estimate D2E/DX2
!
 ! D104  D(17,16,18,12)       -179.1414         estimate D2E/DX2
!
 ! D105  D(17,16,18,19)          0.2582         estimate D2E/DX2
!
 ! D106  D(1,20,22,23)        -179.5194         estimate D2E/DX2
!
 ! D107  D(1,20,22,24)           0.8548         estimate D2E/DX2
!
 ! D108  D(21,20,22,23)          0.3993         estimate D2E/DX2
!
 ! D109  D(21,20,22,24)       -179.2265         estimate D2E/DX2
!
 ! D110  D(20,22,24,25)        179.4299         estimate D2E/DX2
!
 ! D111  D(20,22,24,26)         -0.3118         estimate D2E/DX2
!
 ! D112  D(23,22,24,25)          -0.195          estimate D2E/DX2
!
 ! D113  D(23,22,24,26)       -179.9367         estimate D2E/DX2
!
 ! D114  D(22,24,26,4)          -0.7124         estimate D2E/DX2
!
 ! D115  D(22,24,26,27)        178.6102         estimate D2E/DX2
!
 ! D116  D(25,24,26,4)         179.5444         estimate D2E/DX2
!
 ! D117  D(25,24,26,27)          -1.133          estimate D2E/DX2
!
 ! D118  D(5,28,30,29)           0.9418         estimate D2E/DX2
!
 ! D119  D(32,28,30,29)       -178.3803         estimate D2E/DX2
!
 ! D120  D(10,29,30,28)          -4.1705         estimate D2E/DX2
!
 ! D121  D(31,29,30,28)        175.2948         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ---------------------------------------------------------------------
-----------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
 Number of steps in this run= 210 maximum allowed number of steps=
210.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.625012   -1.036391   -0.390265
      2          6           0       -0.189838   -1.438290   -0.665354
      3          1           0       -0.096854   -2.445603   -1.077914
      4          6           0       -1.752483    0.260069    0.137458
      5          6           0        0.335655   -0.375689   -1.697295
      6          1           0       -0.246091   -0.462633   -2.619280
      7          6           0        0.594594   -1.258902    0.621740
      8          6           0        0.478311    0.025385    1.186827
      9          6           0       -0.396054    0.965644    0.351220
     10          6           0        0.272631    1.029204   -1.071368
     11          1           0       -0.275680    1.757021   -1.675797
     12          6           0        1.390022   -2.227649    1.226706
     13          1           0        1.481670   -3.213968    0.779168
     14          6           0        1.180414    0.335503    2.351041
     15          1           0        1.137452    1.328980    2.785951
     16          6           0        1.968208   -0.645346    2.963800
     17          1           0        2.509369   -0.403810    3.874170
     18          6           0        2.071554   -1.920083    2.408340
     19          1           0        2.689762   -2.673838    2.887561
     20          6           0       -2.754737   -1.806020   -0.647975
     21          1           0       -2.649857   -2.806485   -1.060773
     22          6           0       -4.022608   -1.283546   -0.370561
     23          1           0       -4.907844   -1.883350   -0.562612
     24          6           0       -4.150832    0.006115    0.143607
     25          1           0       -5.136475    0.413669    0.349743
     26          6           0       -3.016385    0.787409    0.393265
     27          1           0       -3.133234    1.797885    0.772341
     28          6           0        1.804026   -0.578812   -2.036786
     29          6           0        1.732677    1.467224   -0.995218
     30          8           0        2.540253    0.519971   -1.616700
     31          8           0        2.197521    2.447357   -0.491015
     32          8           0        2.320973   -1.518264   -2.569480
     33          6           0       -0.613483    2.360055    0.924575
     34          1           0       -0.583271    2.441237    2.030159
     35          8           0       -0.887360    3.320388    0.241538
 ---------------------------------------------------------------------
                   Distance matrix (angstroms):
                   1          2          3          4          5
```

This journal is © The Royal Society of Chemistry 2014

1	C	0.000000				
2	C	1.515560	0.000000			
3	H	2.189522	1.092489	0.000000		
4	C	1.405542	2.443520	3.396895	0.000000	
5	C	2.447258	1.571676	2.203461	2.851461	0.000000
6	H	2.683119	2.184696	2.515999	3.223526	1.093638
7	C	2.449554	1.517934	2.185219	2.837353	2.495003
8	C	2.835235	2.453435	3.400831	2.476428	2.915368
9	C	2.463388	2.618176	3.710600	1.543836	2.555579
10	C	2.886457	2.543079	3.494402	2.480709	1.539312
11	H	3.358041	3.352369	4.248705	2.776636	2.218703
12	C	3.622723	2.588230	2.751287	4.153377	3.618180
13	H	3.969999	2.834363	2.555558	4.789621	3.937264
14	C	4.155390	3.758001	4.596052	3.675258	4.196241
15	H	4.828513	4.618548	5.540798	4.063104	4.862949
16	C	4.930913	4.296124	4.882710	4.759362	4.946084
17	H	5.973163	5.381742	5.956883	5.706762	5.980556
18	C	4.719926	3.846247	4.139098	4.953103	4.717493
19	H	5.660623	4.737286	4.852042	5.992029	5.643068
20	C	1.391051	2.591184	2.767355	2.426961	3.563347
21	H	2.152469	2.842535	2.578440	3.412446	3.902206
22	C	2.410382	3.847203	4.154789	2.791827	4.645308
23	H	3.394706	4.740065	4.871067	3.878227	5.572686
24	C	2.784170	4.293041	4.892624	2.411765	4.864490
25	H	3.870486	5.378605	5.967531	3.394121	5.895563
26	C	2.424064	3.750170	4.597869	1.393188	4.118180
27	H	3.414602	4.604712	5.536266	2.162043	4.780870
28	C	3.831281	2.568077	2.831552	4.252037	1.520732
29	C	4.231800	3.499555	4.320213	3.858305	2.416798
30	O	4.612574	3.491882	4.004904	4.644588	2.380957
31	O	5.172853	4.563785	5.435960	4.558699	3.590438
32	O	4.533429	3.152184	2.988413	5.204135	2.451055
33	C	3.779926	4.139417	5.231751	2.515316	3.906323
34	H	4.363207	4.740391	5.811878	3.115585	4.761660
35	O	4.463724	4.894283	5.967621	3.181953	4.349233

		6	7	8	9	10
6	H	0.000000				
7	C	3.441657	0.000000			
8	C	3.905044	1.407920	0.000000		
9	C	3.299445	2.450137	1.531940	0.000000	
10	C	2.211489	2.864560	2.479799	1.573193	0.000000
11	H	2.412032	3.889967	3.429531	2.179350	1.093479
12	C	4.536932	1.391819	2.430837	3.762135	4.139662
13	H	4.701537	2.152666	3.415600	4.601972	4.784430
14	C	5.232211	2.424004	1.394459	2.623283	3.608071
15	H	5.860085	3.416963	2.165877	2.900270	3.964428
16	C	6.008934	2.783615	2.413981	3.874351	4.686329
17	H	7.054142	3.869864	3.395765	4.767396	5.613811
18	C	5.724736	2.410500	2.795597	4.318362	4.903344
19	H	6.620722	3.394955	3.881857	5.403806	5.935332
20	C	3.461797	3.623470	4.144049	3.774109	4.169258
21	H	3.701443	3.968920	4.780861	4.615442	4.822194

This journal is © The Royal Society of Chemistry 2014

22	C	4.471321	4.722692	4.939335	4.328015	4.928389
23	H	5.289637	5.662989	5.976159	5.413696	5.964824
24	C	4.806274	4.934364	4.745276	3.880999	4.699989
25	H	5.787820	5.976339	5.690105	4.772449	5.626444
26	C	4.279318	4.156773	3.663785	2.626722	3.608496
27	H	4.994860	4.823207	4.044356	2.891733	3.948424
28	C	2.134427	2.998835	3.537549	3.595590	2.421346
29	C	3.205846	3.367722	2.900630	2.568263	1.526235
30	O	3.119998	3.458409	3.515108	3.562756	2.387219
31	O	4.355318	4.188550	3.411273	3.103460	2.460319
32	O	2.776086	3.637518	4.459607	4.699205	3.595781
33	C	4.545487	3.827272	2.590651	1.523284	2.557372
34	H	5.492125	4.130622	2.770290	2.243047	3.513670
35	O	4.786100	4.828109	3.689942	2.407952	2.884237

		11	12	13	14	15
11	H	0.000000				
12	C	5.203526	0.000000			
13	H	5.816001	1.086975	0.000000		
14	C	4.511801	2.806744	3.893621	0.000000	
15	H	4.699719	3.891612	4.978357	1.085352	0.000000
16	C	5.686146	2.419809	3.406928	1.399342	2.149360
17	H	6.574787	3.404173	4.304903	2.152354	2.463521
18	C	5.975849	1.398335	2.162476	2.425919	3.401698
19	H	7.017877	2.155655	2.489287	3.409123	4.294478
20	C	4.460650	4.568504	4.686811	5.391255	6.063762
21	H	5.180787	4.678486	4.541029	6.015275	6.800225
22	C	4.998816	5.721814	5.945207	6.090967	6.589012
23	H	5.995701	6.556166	6.663093	7.104897	7.620862
24	C	4.625225	6.071562	6.519045	5.779571	6.057879
25	H	5.434587	7.095124	7.559365	6.626793	6.792280
26	C	3.568281	5.403852	6.032615	4.652981	4.824169
27	H	3.763066	6.072167	6.812933	4.820624	4.744814
28	C	3.148270	3.679734	3.870085	4.525250	5.229033
29	C	2.140249	4.325095	5.012485	3.575365	3.830228
30	O	3.076242	4.117937	4.561040	4.198352	4.691021
31	O	2.827896	5.045622	5.846059	3.683981	3.621190
32	O	4.274198	3.972521	3.846204	5.380414	6.179657
33	C	2.690668	5.015211	5.956555	3.058052	2.755650
34	H	3.781121	5.132048	6.149008	2.765441	2.183855
35	O	2.548420	6.077643	6.971310	4.199432	3.813084

		16	17	18	19	20
16	C	0.000000				
17	H	1.086264	0.000000			
18	C	1.394335	2.153932	0.000000		
19	H	2.154352	2.481726	1.086269	0.000000	
20	C	6.057912	7.080028	5.713769	6.549480	0.000000
21	H	6.495709	7.532869	5.925553	6.642173	1.087351
22	C	6.885865	7.839541	6.728022	7.589742	1.399083
23	H	7.826131	8.768644	7.585506	8.381657	2.156186
24	C	6.769087	7.644829	6.896183	7.842522	2.420644
25	H	7.644039	8.458652	7.851108	8.787673	3.405163
26	C	5.788489	6.638498	6.105585	7.124736	2.806869

27	H	6.066019	6.804981	6.602242	7.640533	3.892132
28	C	5.003723	5.955463	4.650777	5.424284	4.921093
29	C	4.493579	5.273989	4.813823	5.756768	5.565212
30	O	4.760901	5.568122	4.730168	5.523689	5.863922
31	O	4.642536	5.223145	5.243726	6.154975	6.529986
32	O	5.612808	6.542028	5.000236	5.590228	5.434870
33	C	4.456007	5.107961	5.265982	6.332837	4.941059
34	H	4.112022	4.589019	5.119788	6.132852	5.470545
35	O	5.593928	6.213166	6.396307	7.465118	5.527964

		21	22	23	24	25
21	H	0.000000				
22	C	2.163373	0.000000			
23	H	2.489749	1.086412	0.000000		
24	C	3.407958	1.394287	2.154505	0.000000	
25	H	4.306067	2.154084	2.482128	1.086317	0.000000
26	C	3.894181	2.425854	3.409439	1.399900	2.153220
27	H	4.979376	3.404765	4.299166	2.154356	2.471359
28	C	5.074663	6.101034	6.994584	6.368405	7.406152
29	C	6.121723	6.409387	7.450504	6.168261	7.078428
30	O	6.189637	6.919298	7.896911	6.937820	7.925298
31	O	7.171092	7.254251	8.321440	6.831105	7.657040
32	O	5.352089	6.717988	7.511099	7.181144	8.238189
33	C	5.897589	5.155127	6.217696	4.320160	4.957450
34	H	6.431425	5.609501	6.642774	4.713426	5.259895
35	O	6.506995	5.603629	6.624941	4.652338	5.149340

		26	27	28	29	30
26	C	0.000000				
27	H	1.085548	0.000000			
28	C	5.568489	6.157631	0.000000		
29	C	4.994359	5.187552	2.297002	0.000000	
30	O	5.915041	6.287212	1.387742	1.391297	0.000000
31	O	5.542761	5.516777	3.420811	1.196228	2.258196
32	O	6.525441	7.205067	1.197317	3.426008	2.260592
33	C	2.920521	2.586185	4.821924	3.160256	4.448600
34	H	3.366692	2.915188	5.599993	3.932585	5.171774
35	O	3.312363	2.764727	5.257193	3.439241	4.800408

		31	32	33	34	35
31	O	0.000000				
32	O	4.478996	0.000000			
33	C	3.148533	5.988390	0.000000		
34	H	3.753553	6.728221	1.108972	0.000000	
35	O	3.288664	6.450409	1.209871	2.016071	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

```
 ---------------------------------------------------------------------
     1          6           0       -1.625012   -1.036391   -0.390265
     2          6           0       -0.189838   -1.438290   -0.665354
     3          1           0       -0.096854   -2.445603   -1.077914
     4          6           0       -1.752483    0.260069    0.137458
     5          6           0        0.335655   -0.375689   -1.697295
     6          1           0       -0.246091   -0.462633   -2.619280
     7          6           0        0.594594   -1.258902    0.621740
     8          6           0        0.478311    0.025385    1.186827
     9          6           0       -0.396054    0.965644    0.351220
    10          6           0        0.272631    1.029204   -1.071368
    11          1           0       -0.275680    1.757021   -1.675797
    12          6           0        1.390022   -2.227649    1.226706
    13          1           0        1.481670   -3.213968    0.779168
    14          6           0        1.180414    0.335503    2.351041
    15          1           0        1.137452    1.328980    2.785951
    16          6           0        1.968208   -0.645346    2.963800
    17          1           0        2.509369   -0.403810    3.874170
    18          6           0        2.071554   -1.920083    2.408340
    19          1           0        2.689762   -2.673838    2.887561
    20          6           0       -2.754737   -1.806020   -0.647975
    21          1           0       -2.649857   -2.806485   -1.060773
    22          6           0       -4.022608   -1.283547   -0.370561
    23          1           0       -4.907844   -1.883351   -0.562612
    24          6           0       -4.150832    0.006114    0.143607
    25          1           0       -5.136475    0.413668    0.349743
    26          6           0       -3.016385    0.787409    0.393265
    27          1           0       -3.133234    1.797885    0.772341
    28          6           0        1.804026   -0.578812   -2.036786
    29          6           0        1.732677    1.467224   -0.995218
    30          8           0        2.540253    0.519971   -1.616700
    31          8           0        2.197521    2.447357   -0.491015
    32          8           0        2.320973   -1.518264   -2.569480
    33          6           0       -0.613483    2.360055    0.924575
    34          1           0       -0.583271    2.441237    2.030159
    35          8           0       -0.887360    3.320388    0.241538
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3775167      0.2683587
0.2547946
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1930.9324609525 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
```

```
 NBsUse=   456 1.00D-06 NBFU=   456
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1032.18949692     A.U. after   16 cycles
             Convg  =    0.4422D-08             -V/T =  2.0092

**********************************************************************

            Population analysis using the SCF density.

**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.24037 -19.18464 -19.18126 -19.18001 -
10.35352
 Alpha  occ. eigenvalues --  -10.35304 -10.30702 -10.25713 -10.24933 -
10.24906
 Alpha  occ. eigenvalues --  -10.24263 -10.23192 -10.22831 -10.22668 -
10.22450
 Alpha  occ. eigenvalues --  -10.21982 -10.21934 -10.21888 -10.21741 -
10.21673
 Alpha  occ. eigenvalues --  -10.21647 -10.21504 -10.21446  -1.15781
-1.09298
 Alpha  occ. eigenvalues --   -1.08018  -1.05406  -0.93461  -0.87971
-0.86025
 Alpha  occ. eigenvalues --   -0.82796  -0.80187  -0.77412  -0.76783
-0.75552
 Alpha  occ. eigenvalues --   -0.70955  -0.69191  -0.66589  -0.64937
-0.62811
 Alpha  occ. eigenvalues --   -0.62736  -0.60273  -0.58281  -0.56969
-0.55059
 Alpha  occ. eigenvalues --   -0.54184  -0.52822  -0.50319  -0.49937
-0.48992
 Alpha  occ. eigenvalues --   -0.48596  -0.47852  -0.47307  -0.47021
-0.46265
 Alpha  occ. eigenvalues --   -0.45772  -0.45291  -0.44936  -0.44333
-0.43503
 Alpha  occ. eigenvalues --   -0.43362  -0.41542  -0.40782  -0.40235
-0.40032
 Alpha  occ. eigenvalues --   -0.38346  -0.37706  -0.37050  -0.36853
-0.36248
 Alpha  occ. eigenvalues --   -0.35374  -0.34760  -0.32357  -0.29724
-0.28383
 Alpha  occ. eigenvalues --   -0.27974  -0.27734  -0.27479  -0.26152
 Alpha virt. eigenvalues --   -0.06787  -0.04804  -0.04447  -0.04082
-0.03404
 Alpha virt. eigenvalues --   -0.02113  -0.01915  -0.00785   0.00100
0.00405
 Alpha virt. eigenvalues --    0.00706   0.01953   0.02290   0.03384
0.03599
 Alpha virt. eigenvalues --    0.03813   0.04231   0.04603   0.05388
0.06131
 Alpha virt. eigenvalues --    0.06497   0.06562   0.07263   0.07851
0.07978
 Alpha virt. eigenvalues --    0.08389   0.09405   0.09677   0.09725
0.10166
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.10391   0.11146   0.11349   0.12015
0.12260
 Alpha virt. eigenvalues --    0.12424   0.12911   0.13104   0.13234
0.13470
 Alpha virt. eigenvalues --    0.13768   0.14138   0.14627   0.15007
0.15208
 Alpha virt. eigenvalues --    0.15428   0.15591   0.15754   0.16200
0.16449
 Alpha virt. eigenvalues --    0.16861   0.17202   0.17859   0.18106
0.18323
 Alpha virt. eigenvalues --    0.18743   0.18902   0.19545   0.19683
0.19855
 Alpha virt. eigenvalues --    0.20169   0.20324   0.20708   0.20833
0.21050
 Alpha virt. eigenvalues --    0.21502   0.22004   0.22072   0.22435
0.22566
 Alpha virt. eigenvalues --    0.22956   0.23578   0.23682   0.23783
0.24468
 Alpha virt. eigenvalues --    0.24639   0.24917   0.25230   0.25395
0.25869
 Alpha virt. eigenvalues --    0.26084   0.26401   0.26743   0.27333
0.27923
 Alpha virt. eigenvalues --    0.28234   0.28378   0.28697   0.28909
0.29113
 Alpha virt. eigenvalues --    0.29263   0.30289   0.30790   0.30873
0.31307
 Alpha virt. eigenvalues --    0.31865   0.31998   0.32305   0.32499
0.33045
 Alpha virt. eigenvalues --    0.33261   0.33761   0.34244   0.34810
0.35452
 Alpha virt. eigenvalues --    0.35609   0.35904   0.36410   0.36615
0.37227
 Alpha virt. eigenvalues --    0.37879   0.38154   0.38841   0.39267
0.40122
 Alpha virt. eigenvalues --    0.40897   0.41005   0.41396   0.41513
0.42244
 Alpha virt. eigenvalues --    0.42494   0.43075   0.44398   0.45165
0.45817
 Alpha virt. eigenvalues --    0.46952   0.47961   0.48931   0.51628
0.52776
 Alpha virt. eigenvalues --    0.56269   0.56818   0.58254   0.59408
0.62024
 Alpha virt. eigenvalues --    0.65219   0.66884   0.68105   0.68691
0.69152
 Alpha virt. eigenvalues --    0.70321   0.70577   0.70981   0.71367
0.72324
 Alpha virt. eigenvalues --    0.72778   0.73058   0.73467   0.74428
0.75197
 Alpha virt. eigenvalues --    0.75800   0.76471   0.76901   0.77465
0.78221
 Alpha virt. eigenvalues --    0.79046   0.79873   0.80200   0.80809
0.81267
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.81566   0.83072   0.83499   0.84128
0.84621
 Alpha virt. eigenvalues --    0.85409   0.85923   0.86863   0.88410
0.88885
 Alpha virt. eigenvalues --    0.89750   0.90689   0.91776   0.92108
0.93173
 Alpha virt. eigenvalues --    0.94158   0.94650   0.94924   0.96239
0.97516
 Alpha virt. eigenvalues --    0.98455   0.99040   0.99436   1.00320
1.01688
 Alpha virt. eigenvalues --    1.02718   1.02982   1.04430   1.05452
1.06055
 Alpha virt. eigenvalues --    1.06861   1.08861   1.10883   1.11962
1.12950
 Alpha virt. eigenvalues --    1.14706   1.15767   1.16485   1.16777
1.16914
 Alpha virt. eigenvalues --    1.17889   1.19893   1.21574   1.21982
1.23040
 Alpha virt. eigenvalues --    1.23620   1.24842   1.25556   1.26103
1.26780
 Alpha virt. eigenvalues --    1.29014   1.29323   1.31963   1.32759
1.33204
 Alpha virt. eigenvalues --    1.35256   1.35583   1.36061   1.37077
1.37431
 Alpha virt. eigenvalues --    1.37656   1.38556   1.39645   1.39898
1.40968
 Alpha virt. eigenvalues --    1.41593   1.41829   1.43081   1.43351
1.45104
 Alpha virt. eigenvalues --    1.45647   1.45836   1.48213   1.48856
1.49368
 Alpha virt. eigenvalues --    1.50325   1.50880   1.52583   1.53282
1.56788
 Alpha virt. eigenvalues --    1.57326   1.58854   1.60905   1.62306
1.63918
 Alpha virt. eigenvalues --    1.67220   1.68528   1.70624   1.72013
1.72564
 Alpha virt. eigenvalues --    1.73910   1.76205   1.76496   1.77468
1.78074
 Alpha virt. eigenvalues --    1.80559   1.80790   1.81844   1.82682
1.83464
 Alpha virt. eigenvalues --    1.83594   1.85305   1.86564   1.86650
1.87175
 Alpha virt. eigenvalues --    1.87926   1.89284   1.90222   1.90930
1.92930
 Alpha virt. eigenvalues --    1.94146   1.94291   1.95623   1.96602
1.97553
 Alpha virt. eigenvalues --    1.98379   1.99317   2.00463   2.01874
2.02208
 Alpha virt. eigenvalues --    2.03010   2.03969   2.05532   2.06484
2.07577
 Alpha virt. eigenvalues --    2.08712   2.09989   2.12887   2.13855
2.14150
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    2.16165   2.17609   2.17850   2.19040
2.20386
 Alpha virt. eigenvalues --    2.20617   2.24518   2.26042   2.26708
2.27661
 Alpha virt. eigenvalues --    2.28616   2.29242   2.31211   2.32457
2.33928
 Alpha virt. eigenvalues --    2.36207   2.37088   2.38232   2.40389
2.42435
 Alpha virt. eigenvalues --    2.43563   2.44912   2.48862   2.50850
2.52586
 Alpha virt. eigenvalues --    2.54560   2.57265   2.58098   2.59726
2.59975
 Alpha virt. eigenvalues --    2.63033   2.63574   2.65638   2.68579
2.68843
 Alpha virt. eigenvalues --    2.70047   2.71789   2.72731   2.74328
2.75577
 Alpha virt. eigenvalues --    2.76167   2.79236   2.79912   2.80357
2.82722
 Alpha virt. eigenvalues --    2.83945   2.84621   2.85720   2.88597
2.91425
 Alpha virt. eigenvalues --    2.92565   2.94897   2.99604   3.04598
3.08333
 Alpha virt. eigenvalues --    3.10448   3.14094   3.16878   3.23363
3.24324
 Alpha virt. eigenvalues --    3.27234   3.32787   3.40479   3.41343
4.23724
 Alpha virt. eigenvalues --    4.25285   4.27900   4.31043   4.31921
4.33895
 Alpha virt. eigenvalues --    4.36462   4.39109   4.41453   4.43111
4.45329
 Alpha virt. eigenvalues --    4.49224   4.50032   4.52653   4.56794
4.61662
 Alpha virt. eigenvalues --    4.66823   4.74078   4.75109   4.80120
4.84901
 Alpha virt. eigenvalues --    5.13852   5.39326
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   15.164285  -3.958658  -0.047488   0.312993  -0.720111
0.033076
     2  C   -3.958658  21.510746   0.241520  -7.206596  -1.047523  -
0.024686
     3  H   -0.047488   0.241520   0.528121   0.003335  -0.004496  -
0.002841
     4  C    0.312993  -7.206596   0.003335  27.369865   1.666557
0.016491
     5  C   -0.720111  -1.047523  -0.004496   1.666557  11.983026
0.357430
     6  H    0.033076  -0.024686  -0.002841   0.016491   0.357430
0.478675
     7  C    1.056869  -5.607951  -0.047582  -0.163599   0.260757
0.034898
```

This journal is © The Royal Society of Chemistry 2014

```
     8  C    3.319435  -6.655795  -0.002440  -1.166510   0.585894
0.012280
     9  C   -2.478014   5.463742  -0.007389  -2.739727  -1.690049  -
0.021960
    10  C    1.571596  -1.893455   0.031442  -0.126001  -4.060044  -
0.042532
    11  H   -0.051446  -0.011214  -0.000101   0.074783  -0.028976  -
0.003960
    12  C   -0.959361   2.545509   0.019644  -0.118137   0.049104
0.011354
    13  H   -0.015019  -0.031387   0.003241  -0.003736  -0.015578  -
0.000006
    14  C   -2.329910   1.544803  -0.001122   1.851064   0.361676  -
0.000072
    15  H   -0.000586   0.008230   0.000002  -0.015609   0.003782
0.000000
    16  C   -0.408489   0.197809   0.003214  -0.135459   0.223038  -
0.000258
    17  H    0.001946   0.003209   0.000000  -0.004376   0.000770
0.000000
    18  C   -0.150852  -0.333323   0.009426   0.038091  -0.057382
0.001663
    19  H   -0.003764  -0.018781  -0.000004   0.002550   0.000020
0.000000
    20  C   -1.532959  -0.317805   0.049259  -2.996458   0.018922  -
0.028185
    21  H   -0.037044  -0.069914   0.003370   0.083189   0.007946  -
0.000054
    22  C   -0.883870  -0.791461   0.003656  -0.545610  -0.144234  -
0.004435
    23  H    0.004599  -0.012937  -0.000004   0.026815  -0.001531
0.000002
    24  C    0.741951   0.963758  -0.001339   0.649675   0.229949
0.006561
    25  H    0.000785   0.001381   0.000000   0.022057   0.000955
0.000000
    26  C    0.363485   0.089619   0.013195  -9.275069  -0.433883  -
0.003964
    27  H    0.031882  -0.008726   0.000002  -0.103855  -0.006550  -
0.000001
    28  C   -0.613186   0.901399  -0.017718  -0.617064  -1.126332  -
0.080401
    29  C   -0.364431   0.478179  -0.000891   0.111051   0.757091
0.005876
    30  O   -0.008251   0.142223  -0.000393  -0.009840  -0.405776
0.005874
    31  O    0.031504  -0.049551   0.000080   0.010735  -0.031111  -
0.000646
    32  O    0.015369  -0.093548   0.005167   0.011173  -0.035679  -
0.001711
    33  C   -1.663144  -0.597572   0.005520  -1.092745  -0.440809  -
0.001046
```

34	H	-0.017280	0.040076	0.000000	-0.038355	0.015934	0.000002
35	O	-0.029499	0.034628	0.000016	-0.231162	0.097966	-0.000026

		7	8	9	10	11	12
1	C	1.056869	3.319435	-2.478014	1.571596	-0.051446	-0.959361
2	C	-5.607951	-6.655795	5.463742	-1.893455	-0.011214	2.545509
3	H	-0.047582	-0.002440	-0.007389	0.031442	-0.000101	0.019644
4	C	-0.163599	-1.166510	-2.739727	-0.126001	0.074783	-0.118137
5	C	0.260757	0.585894	-1.690049	-4.060044	-0.028976	0.049104
6	H	0.034898	0.012280	-0.021960	-0.042532	-0.003960	0.011354
7	C	22.740340	9.886163	-5.304954	0.119337	-0.007404	-8.759896
8	C	9.886163	38.740407	-5.739929	-2.570017	0.003214	-8.270673
9	C	-5.304954	-5.739929	19.805152	-0.573029	0.006664	1.321107
10	C	0.119337	-2.570017	-0.573029	14.350649	0.341613	-0.010141
11	H	-0.007404	0.003214	0.006664	0.341613	0.436888	-0.002502
12	C	-8.759896	-8.270673	1.321107	-0.010141	-0.002502	13.486645
13	H	-0.068227	0.052328	0.025045	0.003261	0.000000	0.281102
14	C	-7.203132	-18.545298	2.329976	0.340475	0.027405	6.325859
15	H	0.041969	-0.102588	-0.047954	-0.016430	-0.000003	-0.016417
16	C	0.754022	-0.803695	-0.680425	-0.483957	0.003095	-1.005802
17	H	0.030803	0.031058	-0.019733	-0.001364	0.000000	0.004311
18	C	-1.675378	-0.307617	0.142423	0.063942	-0.000258	1.117337
19	H	0.001829	0.041363	0.000543	0.000409	0.000000	0.003035
20	C	1.458665	-0.318891	-1.283371	0.345896	-0.013125	-0.812388
21	H	0.004454	0.005610	0.003387	-0.000373	0.000000	-0.001195
22	C	0.203454	0.294806	-0.015124	0.109819	-0.004242	-0.307276
23	H	-0.003710	-0.000236	0.003541	0.001304	0.000000	0.000310

This journal is © The Royal Society of Chemistry 2014

24	C	-0.355691	-0.715626	0.011627	-0.346503	0.009976	0.252159
25	H	0.000001	-0.003531	-0.013779	-0.001291	0.000001	-0.000231
26	C	0.973914	1.750668	-0.677933	-0.053018	-0.037372	-0.750365
27	H	0.007400	0.023426	-0.019604	0.015651	-0.000098	0.001029
28	C	-0.909253	-0.523456	1.017828	0.308845	0.020833	0.379546
29	C	-0.413213	-1.023300	-0.130175	-1.271169	-0.074785	0.404536
30	O	-0.168135	-0.141077	0.172956	-0.178302	0.004686	0.012296
31	O	0.051658	0.278775	-0.037361	-0.190736	-0.000636	-0.025671
32	O	0.139828	0.040526	-0.042482	-0.045135	-0.000622	-0.102566
33	C	-0.759580	-1.867802	-2.646748	0.538104	0.013531	0.604875
34	H	-0.006879	-0.150406	-0.106546	-0.017093	0.000175	0.006691
35	O	-0.009680	0.154594	-0.004778	-0.240891	0.005186	-0.006857

		13	14	15	16	17	18
1	C	-0.015019	-2.329910	-0.000586	-0.408489	0.001946	-0.150852
2	C	-0.031387	1.544803	0.008230	0.197809	0.003209	-0.333323
3	H	0.003241	-0.001122	0.000002	0.003214	0.000000	0.009426
4	C	-0.003736	1.851064	-0.015609	-0.135459	-0.004376	0.038091
5	C	-0.015578	0.361676	0.003782	0.223038	0.000770	-0.057382
6	H	-0.000006	-0.000072	0.000000	-0.000258	0.000000	0.001663
7	C	-0.068227	-7.203132	0.041969	0.754022	0.030803	-1.675378
8	C	0.052328	-18.545298	-0.102588	-0.803695	0.031058	-0.307617
9	C	0.025045	2.329976	-0.047954	-0.680425	-0.019733	0.142423
10	C	0.003261	0.340475	-0.016430	-0.483957	-0.001364	0.063942
11	H	0.000000	0.027405	-0.000003	0.003095	0.000000	-0.000258
12	C	0.281102	6.325859	-0.016417	-1.005802	0.004311	1.117337
13	H	0.531695	-0.017459	0.000019	0.008333	-0.000160	0.048386

This journal is © The Royal Society of Chemistry 2014

14	C	-0.017459	23.084829	0.244421	-1.756824	0.022853	-0.196174
15	H	0.000019	0.244421	0.542403	0.147539	-0.004587	0.007813
16	C	0.008333	-1.756824	0.147539	9.194800	0.284526	0.865073
17	H	-0.000160	0.022853	-0.004587	0.284526	0.523654	-0.058140
18	C	0.048386	-0.196174	0.007813	0.865073	-0.058140	6.469421
19	H	-0.004278	0.013477	-0.000168	-0.050893	-0.004191	0.307164
20	C	-0.004500	-0.651732	0.000837	-0.067721	-0.000137	-0.016420
21	H	0.000000	0.000386	0.000000	0.000001	0.000000	0.000489
22	C	-0.000383	-0.280790	0.000103	-0.011907	0.000022	-0.016822
23	H	0.000000	-0.000075	0.000000	-0.000004	0.000000	0.000006
24	C	-0.000117	0.573359	-0.000500	0.064620	-0.000029	0.004606
25	H	0.000000	0.000921	0.000000	0.000059	0.000000	-0.000009
26	C	0.000324	-2.102739	0.002075	-0.014608	0.000480	-0.026814
27	H	0.000000	-0.014256	0.000002	-0.002095	0.000000	0.000072
28	C	0.015771	0.435210	-0.001534	0.033187	-0.001106	-0.055830
29	C	-0.001032	0.387369	0.017138	0.020295	0.001979	0.073907
30	O	-0.000123	0.021756	-0.000148	0.006778	-0.000010	0.001399
31	O	-0.000002	-0.162796	-0.001025	-0.029610	-0.000061	-0.004336
32	O	-0.000249	-0.031562	0.000001	-0.001997	0.000002	-0.006474
33	C	0.002420	1.829419	0.004572	0.005866	0.000024	0.057300
34	H	0.000000	0.103336	0.003477	0.052854	-0.000002	0.000213
35	O	-0.000001	0.018154	0.001689	0.026435	-0.000001	0.000000

		19	20	21	22	23	24
1	C	-0.003764	-1.532959	-0.037044	-0.883870	0.004599	0.741951
2	C	-0.018781	-0.317805	-0.069914	-0.791461	-0.012937	0.963758
3	H	-0.000004	0.049259	0.003370	0.003656	-0.000004	-0.001339

This journal is © The Royal Society of Chemistry 2014

```
     4  C    0.002550  -2.996458   0.083189  -0.545610   0.026815
0.649675
     5  C    0.000020   0.018922   0.007946  -0.144234  -0.001531
0.229949
     6  H    0.000000  -0.028185  -0.000054  -0.004435   0.000002
0.006561
     7  C    0.001829   1.458665   0.004454   0.203454  -0.003710  -
0.355691
     8  C    0.041363  -0.318891   0.005610   0.294806  -0.000236  -
0.715626
     9  C    0.000543  -1.283371   0.003387  -0.015124   0.003541
0.011627
    10  C    0.000409   0.345896  -0.000373   0.109819   0.001304  -
0.346503
    11  H    0.000000  -0.013125   0.000000  -0.004242   0.000000
0.009976
    12  C    0.003035  -0.812388  -0.001195  -0.307276   0.000310
0.252159
    13  H   -0.004278  -0.004500   0.000000  -0.000383   0.000000  -
0.000117
    14  C    0.013477  -0.651732   0.000386  -0.280790  -0.000075
0.573359
    15  H   -0.000168   0.000837   0.000000   0.000103   0.000000  -
0.000500
    16  C   -0.050893  -0.067721   0.000001  -0.011907  -0.000004
0.064620
    17  H   -0.004191  -0.000137   0.000000   0.000022   0.000000  -
0.000029
    18  C    0.307164  -0.016420   0.000489  -0.016822   0.000006
0.004606
    19  H    0.523366   0.000363   0.000000  -0.000022   0.000000
0.000011
    20  C    0.000363   9.854453   0.281122   0.754494   0.001246  -
1.544538
    21  H    0.000000   0.281122   0.534915   0.017266  -0.004271
0.007597
    22  C   -0.000022   0.754494   0.017266   6.864457   0.307298
0.175390
    23  H    0.000000   0.001246  -0.004271   0.307298   0.524577  -
0.034611
    24  C    0.000011  -1.544538   0.007597   0.175390  -0.034611
9.875390
    25  H    0.000000   0.024389  -0.000160  -0.030425  -0.004243
0.332757
    26  C   -0.000258   2.788082  -0.024656   0.605513   0.003728  -
4.432882
    27  H    0.000000  -0.009265   0.000019   0.016865  -0.000158  -
0.020927
    28  C    0.000985  -0.219486   0.001809  -0.014450   0.000017
0.037525
    29  C   -0.001074   0.044809  -0.000503  -0.038040  -0.000069
0.085445
```

This journal is © The Royal Society of Chemistry 2014

30	O	-0.000011	0.014189	0.000000	0.002346	0.000000	-0.000953
31	O	0.000004	0.004030	0.000000	0.000747	0.000000	-0.004302
32	O	-0.000024	0.019688	0.000003	0.000377	0.000000	-0.000838
33	C	-0.000246	0.051351	0.001238	-0.010879	0.000712	-0.313109
34	H	0.000000	-0.004399	0.000000	-0.003145	0.000000	0.039153
35	O	0.000000	0.000762	0.000003	-0.002114	0.000003	0.043419

		25	26	27	28	29	30
1	C	0.000785	0.363485	0.031882	-0.613186	-0.364431	-0.008251
2	C	0.001381	0.089619	-0.008726	0.901399	0.478179	0.142223
3	H	0.000000	0.013195	0.000002	-0.017718	-0.000891	-0.000393
4	C	0.022057	-9.275069	-0.103855	-0.617064	0.111051	-0.009840
5	C	0.000955	-0.433883	-0.006550	-1.126332	0.757091	-0.405776
6	H	0.000000	-0.003964	-0.000001	-0.080401	0.005876	0.005874
7	C	0.000001	0.973914	0.007400	-0.909253	-0.413213	-0.168135
8	C	-0.003531	1.750668	0.023426	-0.523456	-1.023300	-0.141077
9	C	-0.013779	-0.677933	-0.019604	1.017828	-0.130175	0.172956
10	C	-0.001291	-0.053018	0.015651	0.308845	-1.271169	-0.178302
11	H	0.000001	-0.037372	-0.000098	0.020833	-0.074785	0.004686
12	C	-0.000231	-0.750365	0.001029	0.379546	0.404536	0.012296
13	H	0.000000	0.000324	0.000000	0.015771	-0.001032	-0.000123
14	C	0.000921	-2.102739	-0.014256	0.435210	0.387369	0.021756
15	H	0.000000	0.002075	0.000002	-0.001534	0.017138	-0.000148
16	C	0.000059	-0.014608	-0.002095	0.033187	0.020295	0.006778
17	H	0.000000	0.000480	0.000000	-0.001106	0.001979	-0.000010
18	C	-0.000009	-0.026814	0.000072	-0.055830	0.073907	0.001399
19	H	0.000000	-0.000258	0.000000	0.000985	-0.001074	-0.000011

This journal is © The Royal Society of Chemistry 2014

20	C	0.024389	2.788082	-0.009265	-0.219486	0.044809
0.014189						
21	H	-0.000160	-0.024656	0.000019	0.001809	-0.000503
0.000000						
22	C	-0.030425	0.605513	0.016865	-0.014450	-0.038040
0.002346						
23	H	-0.004243	0.003728	-0.000158	0.000017	-0.000069
0.000000						
24	C	0.332757	-4.432882	-0.020927	0.037525	0.085445
-0.000953						
25	H	0.523229	-0.034872	-0.004229	-0.000083	0.000008
0.000000						
26	C	-0.034872	17.452310	0.374228	-0.090879	0.047634
0.017019						
27	H	-0.004229	0.374228	0.521427	-0.000955	0.004251
-0.000002						
28	C	-0.000083	-0.090879	-0.000955	6.690474	-0.874435
0.267285						
29	C	0.000008	0.047634	0.004251	-0.874435	6.774785
0.251744						
30	O	0.000000	0.017019	-0.000002	0.267285	0.251744
8.370692						
31	O	0.000000	-0.000760	-0.000034	0.043164	0.470809
-0.073152						
32	O	0.000000	0.003439	0.000000	0.456354	0.027164
-0.083189						
33	C	-0.001963	-0.315231	-0.001081	0.178692	0.005082
0.012957						
34	H	0.000000	0.033558	-0.001515	0.002348	-0.000150
0.000090						
35	O	0.000025	-0.010118	-0.000660	0.002360	-0.049938
0.001312						

		31	32	33	34	35
1	C	0.031504	0.015369	-1.663144	-0.017280	-0.029499
2	C	-0.049551	-0.093548	-0.597572	0.040076	0.034628
3	H	0.000080	0.005167	0.005520	0.000000	0.000016
4	C	0.010735	0.011173	-1.092745	-0.038355	-0.231162
5	C	-0.031111	-0.035679	-0.440809	0.015934	0.097966
6	H	-0.000646	-0.001711	-0.001046	0.000002	-0.000026
7	C	0.051658	0.139828	-0.759580	-0.006879	-0.009680
8	C	0.278775	0.040526	-1.867802	-0.150406	0.154594
9	C	-0.037361	-0.042482	-2.646748	-0.106546	-0.004778
10	C	-0.190736	-0.045135	0.538104	-0.017093	-0.240891
11	H	-0.000636	-0.000622	0.013531	0.000175	0.005186
12	C	-0.025671	-0.102566	0.604875	0.006691	-0.006857
13	H	-0.000002	-0.000249	0.002420	0.000000	-0.000001
14	C	-0.162796	-0.031562	1.829419	0.103336	0.018154
15	H	-0.001025	0.000001	0.004572	0.003477	0.001689
16	C	-0.029610	-0.001997	0.005866	0.052854	0.026435
17	H	-0.000061	0.000002	0.000024	-0.000002	-0.000001
18	C	-0.004336	-0.006474	0.057300	0.000213	0.000000
19	H	0.000004	-0.000024	-0.000246	0.000000	0.000000

This journal is © The Royal Society of Chemistry 2014

20	C	0.004030	0.019688	0.051351	-0.004399	0.000762
21	H	0.000000	0.000003	0.001238	0.000000	0.000003
22	C	0.000747	0.000377	-0.010879	-0.003145	-0.002114
23	H	0.000000	0.000000	0.000712	0.000000	0.000003
24	C	-0.004302	-0.000838	-0.313109	0.039153	0.043419
25	H	0.000000	0.000000	-0.001963	0.000000	0.000025
26	C	-0.000760	0.003439	-0.315231	0.033558	-0.010118
27	H	-0.000034	0.000000	-0.001081	-0.001515	-0.000660
28	C	0.043164	0.456354	0.178692	0.002348	0.002360
29	C	0.470809	0.027164	0.005082	-0.000150	-0.049938
30	O	-0.073152	-0.083189	0.012957	0.000090	0.001312
31	O	8.050351	0.000273	0.009840	0.000153	0.004760
32	O	0.000273	8.107817	-0.001213	-0.000003	-0.000012
33	C	0.009840	-0.001213	11.487832	0.291237	0.613927
34	H	0.000153	-0.000003	0.291237	0.623067	-0.040582
35	O	0.004760	-0.000012	0.613927	-0.040582	7.870735

Mulliken atomic charges:

		1
1	C	-0.376414
2	C	0.564053
3	H	0.213598
4	C	0.339483
5	C	-0.370756
6	H	0.252602
7	C	-0.302094
8	C	-0.311657
9	C	-0.022928
10	C	-0.020861
11	H	0.288696
12	C	0.323031
13	H	0.190330
14	C	-0.222807
15	H	0.181479
16	C	-0.437798
17	H	0.188258
18	C	-0.302901
19	H	0.188595
20	C	0.108824
21	H	0.185366
22	C	-0.251384
23	H	0.187691
24	C	-0.332962
25	H	0.188250
26	C	-0.233846
27	H	0.197758
28	C	0.352539
29	C	0.274055
30	O	-0.236235
31	O	-0.345093
32	O	-0.379878
33	C	-0.001335
34	H	0.173993

```
    35  O   -0.249653
 Sum of Mulliken atomic charges =   0.00000
 Mulliken charges with hydrogens summed into heavy atoms:
               1
     1  C   -0.376414
     2  C    0.777652
     4  C    0.339483
     5  C   -0.118153
     7  C   -0.302094
     8  C   -0.311657
     9  C   -0.022928
    10  C    0.267835
    12  C    0.513361
    14  C   -0.041328
    16  C   -0.249540
    18  C   -0.114305
    20  C    0.294190
    22  C   -0.063693
    24  C   -0.144712
    26  C   -0.036088
    28  C    0.352539
    29  C    0.274055
    30  O   -0.236235
    31  O   -0.345093
    32  O   -0.379878
    33  C    0.172658
    35  O   -0.249653
 Sum of Mulliken charges with hydrogens summed into heavy atoms =
0.00000
 Electronic spatial extent (au):  <R**2>=           5273.6818
 Charge=              0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=             -4.2090    Y=             -3.0495    Z=
2.0382  Tot=              5.5829
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=           -135.8616   YY=           -141.1520   ZZ=           -
127.4448
   XY=             -0.6607   XZ=             11.6324   YZ=
0.1084
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=             -1.0422   YY=             -6.3325   ZZ=
7.3747
   XY=             -0.6607   XZ=             11.6324   YZ=
0.1084
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=            -66.4072  YYY=            -60.2906  ZZZ=
4.5810  XYY=             -5.4820
  XXY=            -10.9678  XXZ=             30.5835  XZZ=
13.6261  YZZ=             32.3037
  YYZ=              8.2163  XYZ=            -26.9324
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
```

This journal is © The Royal Society of Chemistry 2014

```
 XXXX=          -3281.7578 YYYY=          -2101.9803 ZZZZ=          -
1724.8999 XXXY=             -2.5184
 XXXZ=            45.9851 YYYX=             3.4408 YYYZ=
12.7649 ZZZX=            73.5462
 ZZZY=           -18.8203 XXYY=           -907.6637 XXZZ=           -
903.2440 YYZZ=          -607.8875
 XXYZ=           -10.2075 YYXZ=            46.2661 ZZXY=
16.6293
 N-N= 1.930932460953D+03 E-N=-6.261508903856D+03  KE=
1.022745949311D+03
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6           0.001197381    0.000320309   -0.000113277
      2          6           0.000039685   -0.000295389    0.000207392
      3          1          -0.000187594   -0.000225617    0.000109977
      4          6           0.000919385    0.000045186   -0.000186654
      5          6           0.000326882   -0.000242340   -0.000325014
      6          1          -0.000073258   -0.000032861   -0.000274652
      7          6          -0.000824753    0.000290562   -0.000584174
      8          6          -0.000260042    0.000044390   -0.000335549
      9          6          -0.000181268    0.000417626   -0.000245845
     10          6           0.000549739    0.000264051    0.000166398
     11          1           0.000143507    0.000059436   -0.000683538
     12          6          -0.000177662   -0.000911124   -0.000454860
     13          1           0.000131060   -0.000297865   -0.000148996
     14          6          -0.000524381    0.000889084    0.000310903
     15          1           0.000108125    0.000166164    0.000186733
     16          6           0.000534462    0.000436996    0.001126709
     17          1           0.000192546    0.000072069    0.000185923
     18          6           0.000665260   -0.001024811    0.000517657
     19          1           0.000184273   -0.000158442    0.000096514
     20          6           0.000489618   -0.001049913   -0.000415775
     21          1          -0.000041789   -0.000319586   -0.000129165
     22          6          -0.001173954   -0.000671571   -0.000229358
     23          1          -0.000217766   -0.000121769   -0.000024679
     24          6          -0.001324267    0.000445613    0.000356490
     25          1          -0.000231438    0.000090956    0.000037367
     26          6           0.000312053    0.000979921    0.000515405
     27          1          -0.000355396    0.000198542    0.000116238
     28          6          -0.001979014    0.001662233    0.001563397
     29          6          -0.001404860   -0.000805176   -0.000333871
     30          8           0.000903043   -0.000275696   -0.000531532
     31          8           0.001435514    0.001412755    0.000131797
     32          8           0.001549348   -0.001751271   -0.001659752
     33          6          -0.000142960   -0.002437217    0.002198270
     34          1          -0.000050698    0.000749856   -0.000735702
     35          8          -0.000530781    0.002074899   -0.000414775
```

This journal is © The Royal Society of Chemistry 2014

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.002437217 RMS     0.000760681


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.002782887 RMS     0.000499643
 Search for a local minimum.
 Step number   1 out of a maximum of  210
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Second derivative matrix not updated -- first step.
     Eigenvalues ---    0.00439   0.00458   0.00477   0.00687
0.00782
     Eigenvalues ---    0.01136   0.01168   0.01215   0.01427
0.01475
     Eigenvalues ---    0.01572   0.01800   0.02115   0.02120
0.02129
     Eigenvalues ---    0.02131   0.02132   0.02133   0.02142
0.02143
     Eigenvalues ---    0.02154   0.02157   0.02163   0.02166
0.02827
     Eigenvalues ---    0.03455   0.04142   0.04744   0.05122
0.05299
     Eigenvalues ---    0.05327   0.05712   0.06318   0.06643
0.08153
     Eigenvalues ---    0.08692   0.09361   0.09889   0.12326
0.15998
     Eigenvalues ---    0.15999   0.15999   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16282
0.20162
     Eigenvalues ---    0.21838   0.21998   0.21999   0.22009
0.22565
     Eigenvalues ---    0.22616   0.22636   0.24446   0.24544
0.24585
     Eigenvalues ---    0.24998   0.24999   0.26263   0.27116
0.27761
     Eigenvalues ---    0.28720   0.28872   0.29773   0.29987
0.30052
     Eigenvalues ---    0.32709   0.34396   0.34414   0.34527
0.35121
     Eigenvalues ---    0.35165   0.35231   0.35242   0.35247
0.35248
     Eigenvalues ---    0.35332   0.35355   0.36696   0.39968
0.42013
     Eigenvalues ---    0.42040   0.43403   0.44131   0.44510
0.46029
     Eigenvalues ---    0.46051   0.46077   0.46293   0.46373
0.46769
```

```
     Eigenvalues ---    0.46883   1.00016   1.06183
1.067411000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 RFO step:  Lambda=-2.75603225D-04 EMin= 4.38507065D-03
 Linear search not attempted -- first point.
 Iteration  1 RMS(Cart)=  0.01356142 RMS(Int)=  0.00012194
 Iteration  2 RMS(Cart)=  0.00012153 RMS(Int)=  0.00004636
 Iteration  3 RMS(Cart)=  0.00000002 RMS(Int)=  0.00004636
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.86399  -0.00001   0.00000  -0.00079  -0.00080
2.86319
    R2        2.65609   0.00072   0.00000   0.00173   0.00172
2.65781
    R3        2.62870   0.00143   0.00000   0.00296   0.00296
2.63166
    R4        2.06450   0.00015   0.00000   0.00044   0.00044
2.06494
    R5        2.97004   0.00060   0.00000   0.00220   0.00220
2.97224
    R6        2.86848   0.00027   0.00000   0.00079   0.00079
2.86927
    R7        2.91743   0.00042   0.00000   0.00255   0.00255
2.91998
    R8        2.63274   0.00162   0.00000   0.00347   0.00347
2.63622
    R9        2.06668   0.00027   0.00000   0.00079   0.00079
2.06747
   R10        2.90888   0.00097   0.00000   0.00294   0.00294
2.91182
   R11        2.87377  -0.00003   0.00000  -0.00049  -0.00050
2.87327
   R12        2.66058   0.00087   0.00000   0.00168   0.00170
2.66228
   R13        2.63016   0.00137   0.00000   0.00291   0.00291
2.63307
   R14        2.89495   0.00072   0.00000   0.00222   0.00223
2.89718
   R15        2.63515   0.00128   0.00000   0.00272   0.00272
2.63786
   R16        2.97290   0.00188   0.00000   0.00752   0.00751
2.98042
   R17        2.87859   0.00085   0.00000   0.00283   0.00283
2.88142
   R18        2.06638   0.00034   0.00000   0.00100   0.00100
2.06738
   R19        2.88417   0.00074   0.00000   0.00259   0.00260
2.88677
   R20        2.05409   0.00034   0.00000   0.00097   0.00097
2.05505
   R21        2.64247   0.00143   0.00000   0.00313   0.00313
2.64560
```

This journal is © The Royal Society of Chemistry 2014

R22	2.05102	0.00023	0.00000	0.00064	0.00064
2.05165					
R23	2.64437	0.00138	0.00000	0.00302	0.00302
2.64740					
R24	2.05274	0.00027	0.00000	0.00076	0.00076
2.05350					
R25	2.63491	0.00149	0.00000	0.00323	0.00323
2.63814					
R26	2.05275	0.00026	0.00000	0.00073	0.00073
2.05348					
R27	2.05480	0.00034	0.00000	0.00097	0.00097
2.05576					
R28	2.64388	0.00158	0.00000	0.00344	0.00343
2.64732					
R29	2.05302	0.00025	0.00000	0.00071	0.00071
2.05373					
R30	2.63482	0.00134	0.00000	0.00294	0.00293
2.63775					
R31	2.05284	0.00025	0.00000	0.00071	0.00071
2.05355					
R32	2.64543	0.00158	0.00000	0.00353	0.00353
2.64896					
R33	2.05139	0.00026	0.00000	0.00074	0.00074
2.05213					
R34	2.62245	-0.00002	0.00000	0.00010	0.00010
2.62255					
R35	2.26260	0.00278	0.00000	0.00262	0.00262
2.26522					
R36	2.62917	0.00058	0.00000	0.00161	0.00161
2.63078					
R37	2.26054	0.00177	0.00000	0.00166	0.00166
2.26220					
R38	2.09565	-0.00068	0.00000	-0.00209	-0.00209
2.09357					
R39	2.28632	0.00200	0.00000	0.00200	0.00200
2.28833					
A1	1.98082	0.00030	0.00000	0.00040	0.00040
1.98122					
A2	2.20027	-0.00041	0.00000	-0.00103	-0.00104
2.19923					
A3	2.10161	0.00012	0.00000	0.00074	0.00074
2.10235					
A4	1.97539	-0.00011	0.00000	-0.00201	-0.00202
1.97338					
A5	1.83020	-0.00003	0.00000	-0.00253	-0.00252
1.82768					
A6	1.87981	-0.00014	0.00000	-0.00174	-0.00174
1.87807					
A7	1.92514	-0.00005	0.00000	0.00215	0.00215
1.92729					
A8	1.96621	0.00000	0.00000	-0.00013	-0.00014
1.96607					

A9	1.87974	0.00036	0.00000	0.00436	0.00434
1.88408					
A10	1.97563	-0.00013	0.00000	0.00068	0.00068
1.97631					
A11	2.09480	-0.00008	0.00000	-0.00092	-0.00092
2.09388					
A12	2.21263	0.00021	0.00000	0.00035	0.00033
2.21296					
A13	1.89856	-0.00008	0.00000	-0.00073	-0.00071
1.89785					
A14	1.91387	0.00004	0.00000	0.00091	0.00089
1.91476					
A15	1.95963	0.00028	0.00000	0.00345	0.00344
1.96307					
A16	1.97532	0.00005	0.00000	-0.00153	-0.00154
1.97378					
A17	1.89104	-0.00027	0.00000	-0.00289	-0.00291
1.88813					
A18	1.82576	0.00000	0.00000	0.00090	0.00093
1.82669					
A19	1.98826	0.00007	0.00000	0.00073	0.00073
1.98899					
A20	2.19154	-0.00011	0.00000	-0.00064	-0.00064
2.19090					
A21	2.10326	0.00004	0.00000	-0.00003	-0.00003
2.10323					
A22	1.96935	-0.00005	0.00000	0.00017	0.00016
1.96952					
A23	2.09021	0.00004	0.00000	0.00007	0.00007
2.09028					
A24	2.22216	0.00002	0.00000	0.00003	0.00003
2.22219					
A25	1.87181	-0.00015	0.00000	-0.00351	-0.00351
1.86830					
A26	1.84078	-0.00008	0.00000	0.00060	0.00061
1.84138					
A27	1.92311	-0.00021	0.00000	-0.00385	-0.00389
1.91922					
A28	1.84984	0.00002	0.00000	0.00084	0.00082
1.85066					
A29	2.02418	-0.00023	0.00000	-0.00260	-0.00263
2.02155					
A30	1.94341	0.00064	0.00000	0.00862	0.00864
1.95204					
A31	1.92648	-0.00023	0.00000	-0.00165	-0.00165
1.92482					
A32	1.98585	-0.00012	0.00000	-0.00529	-0.00532
1.98053					
A33	1.81631	-0.00024	0.00000	-0.00194	-0.00190
1.81441					
A34	1.88977	0.00011	0.00000	0.00268	0.00269
1.89247					

This journal is © The Royal Society of Chemistry 2014

A35	1.95314	0.00078	0.00000	0.00982	0.00980
1.96294					
A36	1.89257	-0.00027	0.00000	-0.00347	-0.00352
1.88905					
A37	2.09532	0.00003	0.00000	0.00017	0.00017
2.09549					
A38	2.08604	0.00006	0.00000	0.00038	0.00038
2.08642					
A39	2.10181	-0.00009	0.00000	-0.00055	-0.00055
2.10126					
A40	2.11552	0.00011	0.00000	0.00073	0.00073
2.11625					
A41	2.08652	0.00010	0.00000	0.00045	0.00045
2.08697					
A42	2.08107	-0.00020	0.00000	-0.00121	-0.00121
2.07986					
A43	2.08472	0.00006	0.00000	0.00021	0.00021
2.08493					
A44	2.10377	-0.00011	0.00000	-0.00038	-0.00038
2.10339					
A45	2.09465	0.00005	0.00000	0.00016	0.00016
2.09481					
A46	2.09624	-0.00012	0.00000	-0.00039	-0.00039
2.09585					
A47	2.09157	0.00008	0.00000	0.00029	0.00029
2.09186					
A48	2.09533	0.00005	0.00000	0.00010	0.00010
2.09543					
A49	2.09562	0.00002	0.00000	0.00033	0.00033
2.09595					
A50	2.08590	0.00010	0.00000	0.00028	0.00029
2.08618					
A51	2.10167	-0.00013	0.00000	-0.00061	-0.00062
2.10105					
A52	2.09114	0.00010	0.00000	0.00044	0.00044
2.09158					
A53	2.09656	-0.00014	0.00000	-0.00056	-0.00056
2.09600					
A54	2.09546	0.00005	0.00000	0.00013	0.00013
2.09559					
A55	2.09490	0.00005	0.00000	0.00008	0.00008
2.09498					
A56	2.10304	-0.00012	0.00000	-0.00029	-0.00029
2.10275					
A57	2.08524	0.00007	0.00000	0.00020	0.00021
2.08544					
A58	2.08424	0.00013	0.00000	0.00079	0.00080
2.08503					
A59	2.11076	0.00027	0.00000	0.00172	0.00172
2.11248					
A60	2.08812	-0.00040	0.00000	-0.00251	-0.00251
2.08561					

This journal is © The Royal Society of Chemistry 2014

A61	1.91656	0.00030	0.00000	0.00019	0.00004	1.91661
A62	2.24083	0.00039	0.00000	0.00227	0.00201	2.24284
A63	2.12572	-0.00068	0.00000	-0.00202	-0.00228	2.12344
A64	1.91515	-0.00003	0.00000	-0.00020	-0.00038	1.91477
A65	2.24967	0.00099	0.00000	0.00419	0.00386	2.25353
A66	2.11832	-0.00096	0.00000	-0.00360	-0.00393	2.11439
A67	1.94588	-0.00001	0.00000	-0.00013	0.00000	1.94588
A68	2.02458	0.00046	0.00000	0.00392	0.00388	2.02846
A69	2.14887	0.00076	0.00000	0.00371	0.00368	2.15255
A70	2.10702	-0.00121	0.00000	-0.00653	-0.00657	2.10045
D1	-3.13881	-0.00012	0.00000	-0.00168	-0.00167	-3.14048
D2	-1.03960	-0.00026	0.00000	-0.00182	-0.00180	-1.04140
D3	0.95907	0.00007	0.00000	0.00119	0.00119	0.96026
D4	-0.03077	-0.00001	0.00000	0.00181	0.00181	-0.02896
D5	2.06844	-0.00016	0.00000	0.00167	0.00168	2.07011
D6	-2.21608	0.00017	0.00000	0.00467	0.00467	-2.21141
D7	-0.02641	0.00000	0.00000	-0.00044	-0.00044	-0.02685
D8	3.09883	0.00015	0.00000	0.00670	0.00669	3.10552
D9	-3.13655	-0.00008	0.00000	-0.00367	-0.00367	-3.14022
D10	-0.01131	0.00007	0.00000	0.00347	0.00346	-0.00785
D11	0.03050	-0.00010	0.00000	-0.00353	-0.00353	0.02698
D12	-3.11250	-0.00013	0.00000	-0.00499	-0.00499	-3.11749
D13	3.13641	0.00001	0.00000	0.00016	0.00016	3.13657
D14	-0.00659	-0.00002	0.00000	-0.00130	-0.00130	-0.00789
D15	-1.10353	0.00011	0.00000	0.00918	0.00919	-1.09434
D16	1.06515	0.00014	0.00000	0.00739	0.00739	1.07253

This journal is © The Royal Society of Chemistry 2014

D17	3.08684	0.00033	0.00000	0.01113	0.01115	3.09799
D18	1.02874	-0.00007	0.00000	0.00643	0.00643	1.03517
D19	-3.08576	-0.00004	0.00000	0.00463	0.00462	-3.08114
D20	-1.06408	0.00015	0.00000	0.00837	0.00839	-1.05569
D21	-3.10226	0.00012	0.00000	0.01045	0.01047	-3.09179
D22	-0.93358	0.00016	0.00000	0.00866	0.00866	-0.92492
D23	1.08811	0.00035	0.00000	0.01239	0.01242	1.10054
D24	-0.93621	0.00001	0.00000	0.00026	0.00026	-0.93595
D25	2.22244	-0.00008	0.00000	-0.00423	-0.00423	2.21821
D26	-3.12699	0.00026	0.00000	0.00422	0.00422	-3.12277
D27	0.03166	0.00017	0.00000	-0.00027	-0.00026	0.03139
D28	1.02929	0.00008	0.00000	-0.00141	-0.00141	1.02788
D29	-2.09525	-0.00001	0.00000	-0.00589	-0.00589	-2.10114
D30	-0.92277	-0.00001	0.00000	-0.00085	-0.00085	-0.92362
D31	1.04340	-0.00008	0.00000	-0.00114	-0.00116	1.04225
D32	-3.14054	0.00053	0.00000	0.00743	0.00741	-3.13313
D33	2.23650	-0.00017	0.00000	-0.00855	-0.00855	2.22794
D34	-2.08052	-0.00024	0.00000	-0.00884	-0.00885	-2.08937
D35	0.01872	0.00037	0.00000	-0.00027	-0.00028	0.01844
D36	0.02071	-0.00006	0.00000	-0.00297	-0.00296	0.01774
D37	-3.10891	-0.00007	0.00000	-0.00374	-0.00374	-3.11265
D38	-3.13965	0.00011	0.00000	0.00522	0.00522	-3.13443
D39	0.01393	0.00009	0.00000	0.00445	0.00444	0.01837
D40	-0.07504	-0.00019	0.00000	-0.00917	-0.00917	-0.08421
D41	-2.20358	-0.00007	0.00000	-0.00766	-0.00767	-2.21125
D42	2.02327	0.00048	0.00000	0.00048	0.00047	2.02374

This journal is © The Royal Society of Chemistry 2014

D43	2.04822	-0.00024	0.00000	-0.01049	-0.01049	2.03774
D44	-0.08031	-0.00012	0.00000	-0.00898	-0.00899	-0.08930
D45	-2.13665	0.00043	0.00000	-0.00084	-0.00085	-2.13750
D46	-2.18000	-0.00054	0.00000	-0.01422	-0.01422	-2.19422
D47	1.97465	-0.00042	0.00000	-0.01271	-0.01272	1.96193
D48	-0.08169	0.00013	0.00000	-0.00457	-0.00458	-0.08627
D49	-2.02946	-0.00033	0.00000	-0.00811	-0.00809	-2.03755
D50	1.09930	0.00010	0.00000	0.03100	0.03102	1.13033
D51	2.15654	-0.00021	0.00000	-0.00742	-0.00740	2.14914
D52	-0.99788	0.00022	0.00000	0.03170	0.03172	-0.96616
D53	0.04478	-0.00013	0.00000	-0.00467	-0.00464	0.04014
D54	-3.10965	0.00030	0.00000	0.03445	0.03448	-3.07517
D55	-0.02178	0.00002	0.00000	-0.00258	-0.00258	-0.02436
D56	-3.10940	-0.00013	0.00000	-0.00759	-0.00760	-3.11699
D57	3.10371	0.00010	0.00000	0.00165	0.00165	3.10536
D58	0.01610	-0.00005	0.00000	-0.00337	-0.00337	0.01273
D59	-0.00838	0.00013	0.00000	0.00637	0.00637	-0.00201
D60	3.12910	0.00008	0.00000	0.00480	0.00480	3.13390
D61	-3.13188	0.00003	0.00000	0.00161	0.00161	-3.13027
D62	0.00560	-0.00002	0.00000	0.00004	0.00004	0.00564
D63	0.94584	-0.00001	0.00000	0.00217	0.00216	0.94800
D64	-1.01417	0.00013	0.00000	0.00264	0.00264	-1.01153
D65	3.10281	-0.00056	0.00000	-0.00748	-0.00748	3.09532
D66	-2.25469	0.00016	0.00000	0.00765	0.00765	-2.24704
D67	2.06850	0.00030	0.00000	0.00812	0.00812	2.07662
D68	-0.09772	-0.00039	0.00000	-0.00200	-0.00200	-0.09972

This journal is © The Royal Society of Chemistry 2014

D69	3.10106	0.00004	0.00000	0.00160	0.00160	3.10266
D70	-0.02734	0.00009	0.00000	0.00455	0.00455	-0.02279
D71	0.02204	-0.00014	0.00000	-0.00422	-0.00422	0.01781
D72	-3.10637	-0.00009	0.00000	-0.00127	-0.00127	-3.10763
D73	-0.94345	0.00016	0.00000	0.00747	0.00748	-0.93597
D74	1.24080	-0.00007	0.00000	0.00156	0.00154	1.24234
D75	-2.95746	0.00014	0.00000	0.00497	0.00494	-2.95252
D76	1.03810	-0.00002	0.00000	0.00414	0.00414	1.04224
D77	-3.06084	-0.00025	0.00000	-0.00177	-0.00180	-3.06263
D78	-0.97591	-0.00005	0.00000	0.00164	0.00161	-0.97430
D79	-3.02930	0.00012	0.00000	0.00709	0.00710	-3.02220
D80	-0.84505	-0.00011	0.00000	0.00118	0.00116	-0.84389
D81	1.23987	0.00010	0.00000	0.00459	0.00457	1.24444
D82	1.62317	-0.00014	0.00000	0.01407	0.01408	1.63725
D83	-1.43959	-0.00022	0.00000	-0.00154	-0.00153	-1.44112
D84	-0.50684	0.00040	0.00000	0.02378	0.02377	-0.48307
D85	2.71359	0.00031	0.00000	0.00817	0.00816	2.72175
D86	-2.62379	0.00002	0.00000	0.01765	0.01765	-2.60614
D87	0.59663	-0.00006	0.00000	0.00204	0.00204	0.59867
D88	0.09621	-0.00008	0.00000	0.01253	0.01251	0.10872
D89	-3.03514	-0.00032	0.00000	-0.03166	-0.03171	-3.06685
D90	2.17646	-0.00010	0.00000	0.01442	0.01441	2.19087
D91	-0.95490	-0.00034	0.00000	-0.02976	-0.02980	-0.98470
D92	-2.02345	0.00033	0.00000	0.02147	0.02145	-2.00200
D93	1.12838	0.00009	0.00000	-0.02271	-0.02277	1.10561
D94	-0.01586	0.00005	0.00000	0.00207	0.00207	-0.01379

This journal is © The Royal Society of Chemistry 2014

D95	3.13619	0.00006	0.00000	0.00221	0.00221	3.13839
D96	3.12161	0.00000	0.00000	0.00049	0.00049	3.12210
D97	-0.00953	0.00001	0.00000	0.00063	0.00063	-0.00890
D98	-3.13478	-0.00008	0.00000	-0.00385	-0.00385	-3.13863
D99	0.01725	-0.00006	0.00000	-0.00249	-0.00249	0.01476
D100	0.01974	-0.00003	0.00000	-0.00097	-0.00097	0.01877
D101	-3.11142	-0.00002	0.00000	0.00039	0.00039	-3.11102
D102	0.00449	-0.00001	0.00000	-0.00085	-0.00085	0.00364
D103	3.13560	-0.00002	0.00000	-0.00099	-0.00099	3.13462
D104	-3.12661	0.00001	0.00000	0.00052	0.00052	-3.12609
D105	0.00451	0.00000	0.00000	0.00038	0.00038	0.00489
D106	-3.13320	0.00001	0.00000	0.00072	0.00072	-3.13248
D107	0.01492	-0.00003	0.00000	-0.00132	-0.00132	0.01360
D108	0.00697	-0.00002	0.00000	-0.00075	-0.00074	0.00623
D109	-3.12809	-0.00007	0.00000	-0.00278	-0.00278	-3.13087
D110	3.13164	0.00003	0.00000	0.00150	0.00150	3.13314
D111	-0.00544	0.00004	0.00000	0.00180	0.00180	-0.00365
D112	-0.00340	-0.00001	0.00000	-0.00054	-0.00054	-0.00395
D113	-3.14049	-0.00001	0.00000	-0.00025	-0.00025	-3.14073
D114	-0.01243	0.00001	0.00000	0.00036	0.00036	-0.01208
D115	3.11734	0.00003	0.00000	0.00115	0.00115	3.11849
D116	3.13364	0.00001	0.00000	0.00065	0.00065	3.13429
D117	-0.01977	0.00003	0.00000	0.00145	0.00145	-0.01833
D118	0.01644	0.00010	0.00000	0.01332	0.01330	0.02973
D119	-3.11332	-0.00031	0.00000	-0.02278	-0.02270	-3.13603
D120	-0.07279	-0.00002	0.00000	-0.01652	-0.01650	-0.08929

```
   D121        3.05947   0.00021   0.00000   0.02381   0.02363
3.08310
         Item               Value     Threshold  Converged?
 Maximum Force            0.002783     0.000450     NO
 RMS     Force            0.000500     0.000300     NO
 Maximum Displacement     0.099980     0.001800     NO
 RMS     Displacement     0.013542     0.001200     NO
 Predicted change in Energy=-1.395913D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.619883   -1.034952   -0.392491
      2          6           0       -0.184764   -1.436943   -0.665397
      3          1           0       -0.093299   -2.445678   -1.075426
      4          6           0       -1.748666    0.262740    0.134311
      5          6           0        0.337987   -0.374234   -1.700388
      6          1           0       -0.251096   -0.458396   -2.618460
      7          6           0        0.595744   -1.257161    0.624518
      8          6           0        0.477604    0.027593    1.190395
      9          6           0       -0.392092    0.970260    0.350478
     10          6           0        0.282650    1.032355   -1.073717
     11          1           0       -0.261838    1.759799   -1.682989
     12          6           0        1.386387   -2.228805    1.234637
     13          1           0        1.480862   -3.214893    0.785937
     14          6           0        1.169786    0.334616    2.363062
     15          1           0        1.124704    1.327374    2.800234
     16          6           0        1.954068   -0.648362    2.980552
     17          1           0        2.489895   -0.408102    3.894888
     18          6           0        2.061325   -1.923558    2.422601
     19          1           0        2.676913   -2.678428    2.904305
     20          6           0       -2.749458   -1.808312   -0.648141
     21          1           0       -2.643137   -2.809556   -1.060030
     22          6           0       -4.019887   -1.288690   -0.367919
     23          1           0       -4.904364   -1.891068   -0.557513
     24          6           0       -4.149989    0.001564    0.148496
     25          1           0       -5.136343    0.406607    0.358132
     26          6           0       -3.015058    0.786389    0.395348
     27          1           0       -3.135742    1.795892    0.776931
     28          6           0        1.802009   -0.579999   -2.055536
     29          6           0        1.746453    1.464264   -1.007889
     30          8           0        2.543743    0.520381   -1.649366
     31          8           0        2.220729    2.455952   -0.533886
     32          8           0        2.309371   -1.506364   -2.622387
     33          6           0       -0.617440    2.361396    0.932646
     34          1           0       -0.574810    2.442812    2.036696
     35          8           0       -0.895372    3.327941    0.258186
```

This journal is © The Royal Society of Chemistry 2014

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515137	0.000000			
3	H	2.187922	1.092720	0.000000		
4	C	1.406453	2.444226	3.396944	0.000000	
5	C	2.445486	1.572841	2.206234	2.850610	0.000000
6	H	2.675992	2.185500	2.520942	3.215664	1.094056
7	C	2.447996	1.518352	2.185672	2.836663	2.500238
8	C	2.834428	2.455109	3.402491	2.475255	2.921915
9	C	2.465837	2.620995	3.713639	1.545187	2.558658
10	C	2.890927	2.546101	3.498293	2.485534	1.540866
11	H	3.364566	3.355681	4.252479	2.784676	2.216797
12	C	3.620841	2.589534	2.751889	4.152959	3.626699
13	H	3.969314	2.835805	2.556237	4.790449	3.944277
14	C	4.153438	3.760956	4.598763	3.672855	4.207848
15	H	4.827716	4.622419	5.544384	4.061631	4.875448
16	C	4.929502	4.299930	4.886001	4.758301	4.959643
17	H	5.972004	5.385955	5.960589	5.705906	5.994912
18	C	4.718650	3.849343	4.141401	4.952999	4.729623
19	H	5.659711	4.740596	4.854534	5.992419	5.655359
20	C	1.392616	2.591499	2.764776	2.429624	3.563162
21	H	2.154501	2.843132	2.575717	3.415484	3.902302
22	C	2.413505	3.849499	4.154188	2.796000	4.647879
23	H	3.398232	4.742625	4.870541	3.882775	5.575769
24	C	2.787197	4.295897	4.893231	2.415526	4.868422
25	H	3.873889	5.381860	5.968493	3.398110	5.900467
26	C	2.425797	3.752193	4.598490	1.395027	4.120931
27	H	3.417464	4.608666	5.538827	2.165063	4.786789
28	C	3.831716	2.571791	2.834355	4.255929	1.520470
29	C	4.237572	3.501985	4.321677	3.868350	2.417313
30	O	4.618937	3.499152	4.010101	4.655390	2.380819
31	O	5.191985	4.578026	5.447382	4.583968	3.593799
32	O	4.542434	3.171016	3.008027	5.215053	2.453193
33	C	3.781013	4.143468	5.235937	2.514233	3.915275
34	H	4.368979	4.744043	5.815023	3.122455	4.768097
35	O	4.470250	4.905312	5.979675	3.184166	4.366152

		6	7	8	9	10
6	H	0.000000				
7	C	3.445587	0.000000			
8	C	3.908269	1.408818	0.000000		
9	C	3.297807	2.452004	1.533119	0.000000	
10	C	2.212115	2.867736	2.484704	1.577170	0.000000
11	H	2.407407	3.893852	3.435643	2.185251	1.094009
12	C	4.545553	1.393360	2.432935	3.765467	4.145105
13	H	4.710401	2.154578	3.418161	4.605767	4.788855
14	C	5.240547	2.426070	1.395897	2.625644	3.617361
15	H	5.868905	3.419556	2.167891	2.903362	3.975373
16	C	6.020612	2.786858	2.416924	3.878362	4.696332
17	H	7.066771	3.873504	3.399033	4.771643	5.624400
18	C	5.736400	2.413528	2.798838	4.322862	4.911755

This journal is © The Royal Society of Chemistry 2014

19	H	6.633454	3.398337	3.885485	5.408674	5.943657
20	C	3.456334	3.621298	4.143029	3.778210	4.176623
21	H	3.698448	3.967113	4.780466	4.619929	4.829151
22	C	4.467450	4.721226	4.938458	4.333572	4.939355
23	H	5.287056	5.661291	5.975117	5.419616	5.976452
24	C	4.803017	4.932845	4.743506	3.885995	4.712178
25	H	5.785669	5.974604	5.687944	4.777622	5.639790
26	C	4.274578	4.155299	3.661497	2.629786	3.618499
27	H	4.993163	4.823728	4.044021	2.896747	3.961476
28	C	2.132349	3.016010	3.557989	3.606423	2.423242
29	C	3.206363	3.375654	2.916582	2.581196	1.527612
30	O	3.115810	3.482084	3.546268	3.580628	2.388730
31	O	4.353021	4.215410	3.450878	3.133084	2.464588
32	O	2.766631	3.679812	4.499523	4.719057	3.598759
33	C	4.549262	3.828931	2.590790	1.524782	2.569437
34	H	5.494750	4.129679	2.767144	2.246136	3.521264
35	O	4.798596	4.835368	3.694100	2.412564	2.903690

		11	12	13	14	15
11	H	0.000000				
12	C	5.209428	0.000000			
13	H	5.820667	1.087486	0.000000		
14	C	4.522302	2.809161	3.896551	0.000000	
15	H	4.712619	3.894353	4.981609	1.085689	0.000000
16	C	5.697200	2.422453	3.409888	1.400941	2.150324
17	H	6.586694	3.407290	4.308340	2.154253	2.464526
18	C	5.984987	1.399991	2.164059	2.428526	3.404178
19	H	7.026904	2.157640	2.491147	3.412156	4.297282
20	C	4.471082	4.563647	4.683018	5.387018	6.060771
21	H	5.190151	4.673311	4.536438	6.011802	6.797975
22	C	5.014542	5.716625	5.941371	6.084907	6.583905
23	H	6.012369	6.549764	6.657964	7.097798	7.614624
24	C	4.643646	6.066770	6.516012	5.771935	6.050775
25	H	5.455099	7.089404	7.555507	6.617567	6.783243
26	C	3.584304	5.400789	6.031262	4.646388	4.818068
27	H	3.783098	6.071023	6.813302	4.815466	4.739690
28	C	3.142119	3.703585	3.888415	4.556340	5.260734
29	C	2.139236	4.335588	5.018252	3.601660	3.860972
30	O	3.067340	4.149093	4.583960	4.245215	4.739605
31	O	2.822801	5.076489	5.869226	3.741237	3.686640
32	O	4.261620	4.031186	3.901560	5.435308	6.232041
33	C	2.707382	5.017615	5.959815	3.057467	2.755386
34	H	3.794801	5.129678	6.148155	2.755834	2.171529
35	O	2.574605	6.085828	6.980952	4.201830	3.813789

		16	17	18	19	20
16	C	0.000000				
17	H	1.086668	0.000000			
18	C	1.396044	2.155901	0.000000		
19	H	2.156267	2.484071	1.086654	0.000000	
20	C	6.052772	7.074639	5.708447	6.543888	0.000000
21	H	6.490867	7.527697	5.919939	6.635969	1.087864
22	C	6.878256	7.830978	6.720952	7.581949	1.400900
23	H	7.816669	8.757747	7.576474	8.371373	2.158398

This journal is © The Royal Society of Chemistry 2014

24	C	6.760359	7.634876	6.888982	7.834758	2.423173
25	H	7.633083	8.445821	7.842074	8.777665	3.408177
26	C	5.782215	6.631599	6.101085	7.120278	2.809250
27	H	6.061063	6.799047	6.599397	7.637553	3.894911
28	C	5.038847	5.992519	4.682532	5.456087	4.919895
29	C	4.518180	5.300535	4.831639	5.773466	5.572466
30	O	4.811426	5.621720	4.773518	5.566510	5.868836
31	O	4.696716	5.281031	5.286428	6.196056	6.549791
32	O	5.679378	6.611629	5.068282	5.661550	5.438802
33	C	4.457041	5.108867	5.268451	6.335615	4.942757
34	H	4.103832	4.579629	5.115009	6.128095	5.478093
35	O	5.598354	6.216402	6.403514	7.472592	5.535355

		21	22	23	24	25
21	H	0.000000				
22	C	2.165062	0.000000			
23	H	2.491845	1.086787	0.000000		
24	C	3.410797	1.395839	2.156290	0.000000	
25	H	4.309404	2.155842	2.484256	1.086692	0.000000
26	C	3.897085	2.428623	3.412652	1.401768	2.155334
27	H	4.982694	3.406911	4.301446	2.154818	2.471419
28	C	5.071616	6.102850	6.995600	6.373559	7.412146
29	C	6.126725	6.421759	7.462872	6.184233	7.096304
30	O	6.191892	6.927921	7.904526	6.950362	7.938937
31	O	7.187461	7.279779	8.346502	6.861174	7.689084
32	O	5.354121	6.722315	7.513300	7.188531	8.245096
33	C	5.900250	5.156669	6.219464	4.320023	4.956989
34	H	6.438561	5.619150	6.652630	4.723018	5.269848
35	O	6.516230	5.609624	6.631398	4.655034	5.150730

		26	27	28	29	30
26	C	0.000000				
27	H	1.085940	0.000000			
28	C	5.574764	6.168396	0.000000		
29	C	5.010047	5.208780	2.297751	0.000000	
30	O	5.928903	6.306378	1.387796	1.392150	0.000000
31	O	5.573543	5.553891	3.421658	1.197106	2.257226
32	O	6.535518	7.218692	1.198703	3.427552	2.260397
33	C	2.918545	2.585708	4.840947	3.187242	4.477634
34	H	3.375289	2.926412	5.615427	3.951622	5.196939
35	O	3.312306	2.763246	5.282155	3.472099	4.832045

		31	32	33	34	35
31	O	0.000000				
32	O	4.479915	0.000000			
33	C	3.196070	6.013656	0.000000		
34	H	3.797776	6.754373	1.107869	0.000000	
35	O	3.331340	6.476001	1.210931	2.012291	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

This journal is © The Royal Society of Chemistry 2014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.620634	-1.023935	-0.418939
2	6	0	-0.184453	-1.428041	-0.682989
3	1	0	-0.092880	-2.431426	-1.105919
4	6	0	-1.749548	0.266929	0.124349
5	6	0	0.352895	-0.353395	-1.697987
6	1	0	-0.227260	-0.422536	-2.622972
7	6	0	0.583758	-1.269178	0.617015
8	6	0	0.465042	0.008169	1.199301
9	6	0	-0.392415	0.965835	0.363778
10	6	0	0.296851	1.044681	-1.052611
11	1	0	-0.238590	1.782646	-1.657231
12	6	0	1.364361	-2.252340	1.221584
13	1	0	1.459423	-3.232562	0.760329
14	6	0	1.146616	0.296232	2.382942
15	1	0	1.101087	1.283078	2.833256
16	6	0	1.920739	-0.698339	2.994661
17	1	0	2.448299	-0.472846	3.917526
18	6	0	2.028531	-1.966192	2.420322
19	1	0	2.636241	-2.730123	2.897726
20	6	0	-2.750646	-1.789064	-0.696481
21	1	0	-2.644170	-2.784994	-1.121021
22	6	0	-4.021753	-1.268116	-0.421852
23	1	0	-4.906666	-1.864195	-0.628547
24	6	0	-4.151911	0.015458	0.110936
25	1	0	-5.138705	0.421639	0.316253
26	6	0	-3.016409	0.792151	0.379892
27	1	0	-3.136910	1.796813	0.774101
28	6	0	1.819584	-0.560288	-2.041279
29	6	0	1.761623	1.469625	-0.966218
30	8	0	2.561564	0.531359	-1.612617
31	8	0	2.235047	2.452761	-0.473902
32	8	0	2.328933	-1.480870	-2.615719
33	6	0	-0.618074	2.349770	0.962746
34	1	0	-0.586220	2.415861	2.068183
35	8	0	-0.885369	3.326609	0.298900

Rotational constants (GHZ): 0.3739180 0.2668334 0.2546663
Standard basis: 6-31+G(d) (6D, 7F)
There are 461 symmetry adapted basis functions of A symmetry.
Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
461 basis functions, 784 primitive gaussians, 461 cartesian basis functions
79 alpha electrons 79 beta electrons
nuclear repulsion energy 1927.1566869420 Hartrees.

This journal is © The Royal Society of Chemistry 2014

```
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
```

```
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1032.18951147     A.U. after   14 cycles
             Convg  =    0.7235D-08             -V/T =  2.0093
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6          -0.000377029    0.000222828    0.000097927
      2          6          -0.000112386    0.000149365   -0.000022580
      3          1           0.000002389   -0.000004185   -0.000014047
      4          6          -0.000313365   -0.000185302   -0.000119128
      5          6           0.000452023   -0.001064426    0.001234785
      6          1           0.000177944   -0.000147077   -0.000012936
      7          6           0.000097376    0.000185087   -0.000102744
      8          6           0.000304853   -0.000035108   -0.000026949
      9          6          -0.000720807    0.000274276   -0.000488398
     10          6           0.000193013   -0.000689349    0.002120953
     11          1           0.000307233    0.000190922   -0.000102951
     12          6          -0.000025642    0.000082325   -0.000015594
     13          1           0.000009122    0.000006931    0.000020959
     14          6           0.000075395   -0.000043527   -0.000153006
     15          1           0.000067295   -0.000090453    0.000050958
     16          6          -0.000052665   -0.000020640   -0.000054879
     17          1          -0.000039298   -0.000012124   -0.000035418
     18          6          -0.000065081   -0.000011814   -0.000008823
     19          1          -0.000027040    0.000026707   -0.000028591
     20          6           0.000071198    0.000035394    0.000071276
     21          1          -0.000009968    0.000045470    0.000003600
     22          6           0.000045936    0.000021295    0.000041666
     23          1           0.000041055    0.000024140   -0.000007533
     24          6           0.000096774   -0.000045954   -0.000001767
     25          1           0.000061343    0.000009614    0.000007723
     26          6           0.000143915   -0.000064025   -0.000027797
     27          1          -0.000086680   -0.000024509   -0.000040279
```

This journal is © The Royal Society of Chemistry 2014

```
     28        6          -0.000921270    0.002261616   -0.002929973
     29        6          -0.000840519    0.002421813   -0.003274594
     30        8           0.000291897   -0.001456707    0.001728213
     31        8           0.000111539   -0.000683489    0.001331123
     32        8           0.000370693   -0.000948668    0.000956009
     33        6           0.001677182   -0.000447101    0.000355121
     34        1          -0.000533360   -0.000112398   -0.000181555
     35        8          -0.000473066    0.000129073   -0.000370771
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.003274594 RMS     0.000721521


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000853453 RMS     0.000212423
 Search for a local minimum.
 Step number   2 out of a maximum of  210
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2
 DE= -1.46D-05 DEPred=-1.40D-04 R= 1.04D-01
 Trust test= 1.04D-01 RLast= 1.12D-01 DXMaxT set to 3.00D-01
     Eigenvalues ---    0.00425   0.00455   0.00482   0.00766
0.01090
     Eigenvalues ---    0.01104   0.01162   0.01424   0.01475
0.01568
     Eigenvalues ---    0.01800   0.01873   0.02115   0.02122
0.02129
     Eigenvalues ---    0.02131   0.02133   0.02136   0.02143
0.02151
     Eigenvalues ---    0.02155   0.02158   0.02165   0.02178
0.02923
     Eigenvalues ---    0.03444   0.04163   0.04717   0.05039
0.05232
     Eigenvalues ---    0.05334   0.05709   0.06285   0.06647
0.08020
     Eigenvalues ---    0.08615   0.09331   0.09792   0.12403
0.15587
     Eigenvalues ---    0.15998   0.15999   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16011   0.16368
0.20183
     Eigenvalues ---    0.21335   0.21997   0.21999   0.22072
0.22522
     Eigenvalues ---    0.22608   0.22635   0.24108   0.24550
0.24571
     Eigenvalues ---    0.24795   0.24989   0.26445   0.27081
0.27644
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.28741   0.28832   0.29714   0.29971
0.30295
     Eigenvalues ---    0.32571   0.34375   0.34403   0.34523
0.35096
     Eigenvalues ---    0.35149   0.35223   0.35237   0.35244
0.35248
     Eigenvalues ---    0.35326   0.35355   0.36707   0.39999
0.41996
     Eigenvalues ---    0.42044   0.42686   0.43545   0.44146
0.45393
     Eigenvalues ---    0.46050   0.46110   0.46235   0.46336
0.46459
     Eigenvalues ---    0.46831   0.98774   1.04509
1.066511000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     2    1
 RFO step:  Lambda=-5.13184431D-05.
 DIIS coeffs:      0.52933      0.47067
 Iteration  1 RMS(Cart)=  0.00846974 RMS(Int)=  0.00013744
 Iteration  2 RMS(Cart)=  0.00012311 RMS(Int)=  0.00006986
 Iteration  3 RMS(Cart)=  0.00000002 RMS(Int)=  0.00006986
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86319   0.00012   0.00038  -0.00066  -0.00029
2.86290
    R2        2.65781  -0.00025  -0.00081   0.00181   0.00100
2.65881
    R3        2.63166  -0.00018  -0.00139   0.00349   0.00210
2.63377
    R4        2.06494   0.00001  -0.00021   0.00056   0.00036
2.06530
    R5        2.97224  -0.00026  -0.00104   0.00236   0.00133
2.97356
    R6        2.86927  -0.00025  -0.00037   0.00041   0.00004
2.86931
    R7        2.91998   0.00019  -0.00120   0.00337   0.00217
2.92215
    R8        2.63622  -0.00017  -0.00164   0.00413   0.00250
2.63872
    R9        2.06747  -0.00008  -0.00037   0.00087   0.00050
2.06797
   R10        2.91182   0.00036  -0.00138   0.00419   0.00282
2.91464
   R11        2.87327  -0.00029   0.00023  -0.00131  -0.00111
2.87216
   R12        2.66228  -0.00024  -0.00080   0.00186   0.00105
2.66333
   R13        2.63307  -0.00012  -0.00137   0.00350   0.00212
2.63519
   R14        2.89718   0.00008  -0.00105   0.00313   0.00208
2.89925
```

R15	2.63786	-0.00007	-0.00128	0.00332	0.00204
2.63990					
R16	2.98042	-0.00068	-0.00354	0.00785	0.00433
2.98474					
R17	2.88142	-0.00057	-0.00133	0.00254	0.00121
2.88263					
R18	2.06738	0.00003	-0.00047	0.00130	0.00083
2.06820					
R19	2.88677	-0.00030	-0.00122	0.00282	0.00163
2.88839					
R20	2.05505	-0.00002	-0.00045	0.00118	0.00073
2.05578					
R21	2.64560	-0.00017	-0.00147	0.00372	0.00224
2.64784					
R22	2.05165	-0.00006	-0.00030	0.00070	0.00040
2.05206					
R23	2.64740	-0.00010	-0.00142	0.00367	0.00225
2.64965					
R24	2.05350	-0.00005	-0.00036	0.00088	0.00052
2.05402					
R25	2.63814	-0.00013	-0.00152	0.00390	0.00238
2.64052					
R26	2.05348	-0.00005	-0.00034	0.00084	0.00050
2.05397					
R27	2.05576	-0.00004	-0.00046	0.00115	0.00069
2.05646					
R28	2.64732	-0.00014	-0.00162	0.00414	0.00252
2.64984					
R29	2.05373	-0.00004	-0.00033	0.00082	0.00048
2.05421					
R30	2.63775	-0.00011	-0.00138	0.00356	0.00217
2.63993					
R31	2.05355	-0.00005	-0.00033	0.00081	0.00048
2.05403					
R32	2.64896	-0.00013	-0.00166	0.00426	0.00260
2.65156					
R33	2.05213	-0.00003	-0.00035	0.00088	0.00053
2.05266					
R34	2.62255	-0.00015	-0.00005	-0.00001	-0.00008
2.62248					
R35	2.26522	0.00044	-0.00123	0.00349	0.00226
2.26748					
R36	2.63078	0.00033	-0.00076	0.00252	0.00178
2.63256					
R37	2.26220	0.00001	-0.00078	0.00208	0.00130
2.26350					
R38	2.09357	-0.00021	0.00098	-0.00295	-0.00197
2.09160					
R39	2.28833	0.00042	-0.00094	0.00273	0.00178
2.29011					
A1	1.98122	-0.00004	-0.00019	0.00052	0.00033
1.98155					

This journal is © The Royal Society of Chemistry 2014

A2	2.19923	-0.00005	0.00049	-0.00144	-0.00095
2.19828					
A3	2.10235	0.00009	-0.00035	0.00104	0.00070
2.10305					
A4	1.97338	-0.00002	0.00095	-0.00257	-0.00162
1.97176					
A5	1.82768	0.00008	0.00119	-0.00237	-0.00119
1.82649					
A6	1.87807	0.00008	0.00082	-0.00184	-0.00102
1.87706					
A7	1.92729	0.00002	-0.00101	0.00262	0.00160
1.92889					
A8	1.96607	-0.00004	0.00006	-0.00030	-0.00024
1.96583					
A9	1.88408	-0.00012	-0.00204	0.00457	0.00253
1.88661					
A10	1.97631	-0.00002	-0.00032	0.00056	0.00024
1.97655					
A11	2.09388	-0.00002	0.00043	-0.00113	-0.00069
2.09319					
A12	2.21296	0.00004	-0.00016	0.00065	0.00049
2.21344					
A13	1.89785	-0.00010	0.00033	-0.00157	-0.00125
1.89660					
A14	1.91476	-0.00005	-0.00042	0.00098	0.00057
1.91533					
A15	1.96307	0.00022	-0.00162	0.00528	0.00366
1.96672					
A16	1.97378	0.00013	0.00073	-0.00069	0.00005
1.97383					
A17	1.88813	-0.00010	0.00137	-0.00451	-0.00312
1.88500					
A18	1.82669	-0.00009	-0.00044	0.00069	0.00023
1.82692					
A19	1.98899	0.00009	-0.00034	0.00083	0.00049
1.98948					
A20	2.19090	-0.00017	0.00030	-0.00099	-0.00069
2.19021					
A21	2.10323	0.00008	0.00001	0.00022	0.00023
2.10346					
A22	1.96952	-0.00009	-0.00008	0.00011	0.00003
1.96955					
A23	2.09028	-0.00008	-0.00003	-0.00017	-0.00020
2.09008					
A24	2.22219	0.00017	-0.00001	0.00040	0.00038
2.22256					
A25	1.86830	0.00004	0.00165	-0.00353	-0.00188
1.86641					
A26	1.84138	0.00014	-0.00029	0.00097	0.00068
1.84207					
A27	1.91922	0.00004	0.00183	-0.00416	-0.00233
1.91688					

This journal is © The Royal Society of Chemistry 2014

A28	1.85066	-0.00004	-0.00039	0.00047	0.00010
1.85076					
A29	2.02155	0.00004	0.00124	-0.00342	-0.00218
2.01936					
A30	1.95204	-0.00021	-0.00407	0.00973	0.00566
1.95770					
A31	1.92482	-0.00007	0.00078	-0.00212	-0.00136
1.92346					
A32	1.98053	0.00010	0.00250	-0.00590	-0.00338
1.97715					
A33	1.81441	0.00013	0.00089	-0.00121	-0.00032
1.81409					
A34	1.89247	0.00001	-0.00127	0.00346	0.00218
1.89465					
A35	1.96294	0.00009	-0.00461	0.01246	0.00784
1.97078					
A36	1.88905	-0.00025	0.00166	-0.00663	-0.00497
1.88408					
A37	2.09549	0.00002	-0.00008	0.00031	0.00023
2.09571					
A38	2.08642	0.00001	-0.00018	0.00043	0.00025
2.08667					
A39	2.10126	-0.00003	0.00026	-0.00074	-0.00048
2.10078					
A40	2.11625	0.00010	-0.00034	0.00124	0.00090
2.11715					
A41	2.08697	0.00001	-0.00021	0.00061	0.00039
2.08736					
A42	2.07986	-0.00011	0.00057	-0.00188	-0.00131
2.07855					
A43	2.08493	-0.00002	-0.00010	0.00019	0.00009
2.08502					
A44	2.10339	0.00002	0.00018	-0.00039	-0.00021
2.10318					
A45	2.09481	0.00000	-0.00007	0.00018	0.00011
2.09492					
A46	2.09585	-0.00005	0.00018	-0.00061	-0.00043
2.09542					
A47	2.09186	0.00002	-0.00014	0.00041	0.00027
2.09213					
A48	2.09543	0.00003	-0.00005	0.00020	0.00015
2.09558					
A49	2.09595	0.00002	-0.00015	0.00046	0.00031
2.09625					
A50	2.08618	-0.00004	-0.00013	0.00028	0.00014
2.08633					
A51	2.10105	0.00002	0.00029	-0.00074	-0.00045
2.10060					
A52	2.09158	0.00001	-0.00021	0.00054	0.00033
2.09191					
A53	2.09600	-0.00004	0.00026	-0.00076	-0.00050
2.09551					

```
   A54        2.09559   0.00003  -0.00006   0.00023   0.00017
2.09576
   A55        2.09498   0.00002  -0.00004   0.00017   0.00013
2.09511
   A56        2.10275   0.00003   0.00014  -0.00027  -0.00014
2.10261
   A57        2.08544  -0.00005  -0.00010   0.00010   0.00000
2.08545
   A58        2.08503  -0.00003  -0.00037   0.00088   0.00051
2.08554
   A59        2.11248   0.00011  -0.00081   0.00252   0.00171
2.11419
   A60        2.08561  -0.00008   0.00118  -0.00339  -0.00221
2.08340
   A61        1.91661   0.00007  -0.00002   0.00065   0.00033
1.91694
   A62        2.24284  -0.00004  -0.00094   0.00265   0.00149
2.24433
   A63        2.12344  -0.00001   0.00107  -0.00260  -0.00175
2.12169
   A64        1.91477  -0.00016   0.00018   0.00031   0.00017
1.91494
   A65        2.25353   0.00005  -0.00182   0.00511   0.00293
2.25646
   A66        2.11439   0.00016   0.00185  -0.00434  -0.00285
2.11154
   A67        1.94588   0.00011   0.00000   0.00108   0.00105
1.94694
   A68        2.02846   0.00016  -0.00183   0.00383   0.00162
2.03007
   A69        2.15255  -0.00035  -0.00173   0.00287   0.00075
2.15330
   A70        2.10045   0.00016   0.00309  -0.00924  -0.00655
2.09390
    D1       -3.14048  -0.00001   0.00079  -0.00180  -0.00102  -
3.14150
    D2       -1.04140   0.00005   0.00085  -0.00156  -0.00073  -
1.04213
    D3        0.96026  -0.00001  -0.00056   0.00171   0.00115
0.96141
    D4       -0.02896   0.00001  -0.00085   0.00306   0.00221  -
0.02676
    D5        2.07011   0.00007  -0.00079   0.00330   0.00250
2.07262
    D6       -2.21141   0.00001  -0.00220   0.00657   0.00437  -
2.20703
    D7       -0.02685   0.00000   0.00021  -0.00075  -0.00054  -
0.02739
    D8        3.10552   0.00001  -0.00315   0.00830   0.00516
3.11068
    D9       -3.14022  -0.00001   0.00173  -0.00526  -0.00354
3.13942
```

This journal is © The Royal Society of Chemistry 2014

D10	-0.00785	-0.00001	-0.00163	0.00379	0.00216	-0.00569
D11	0.02698	-0.00002	0.00166	-0.00491	-0.00325	0.02373
D12	-3.11749	-0.00002	0.00235	-0.00655	-0.00420	-3.12169
D13	3.13657	0.00000	-0.00008	0.00026	0.00018	3.13675
D14	-0.00789	0.00000	0.00061	-0.00139	-0.00077	-0.00867
D15	-1.09434	-0.00009	-0.00433	0.00896	0.00462	-1.08972
D16	1.07253	-0.00002	-0.00348	0.00769	0.00423	1.07676
D17	3.09799	-0.00003	-0.00525	0.01234	0.00708	3.10507
D18	1.03517	-0.00006	-0.00303	0.00587	0.00284	1.03800
D19	-3.08114	0.00001	-0.00217	0.00460	0.00244	-3.07871
D20	-1.05569	0.00000	-0.00395	0.00925	0.00529	-1.05040
D21	-3.09179	-0.00017	-0.00493	0.01019	0.00525	-3.08654
D22	-0.92492	-0.00010	-0.00408	0.00892	0.00485	-0.92007
D23	1.10054	-0.00011	-0.00585	0.01357	0.00771	1.10824
D24	-0.93595	-0.00002	-0.00012	-0.00037	-0.00050	-0.93645
D25	2.21821	-0.00005	0.00199	-0.00613	-0.00414	2.21407
D26	-3.12277	-0.00002	-0.00199	0.00448	0.00249	-3.12028
D27	0.03139	-0.00005	0.00012	-0.00128	-0.00116	0.03024
D28	1.02788	0.00006	0.00066	-0.00182	-0.00115	1.02673
D29	-2.10114	0.00003	0.00277	-0.00757	-0.00480	-2.10594
D30	-0.92362	0.00005	0.00040	-0.00037	0.00003	-0.92359
D31	1.04225	0.00009	0.00054	-0.00092	-0.00036	1.04189
D32	-3.13313	-0.00006	-0.00349	0.00902	0.00553	-3.12760
D33	2.22794	0.00004	0.00403	-0.01015	-0.00613	2.22181
D34	-2.08937	0.00008	0.00417	-0.01070	-0.00652	-2.09589
D35	0.01844	-0.00007	0.00013	-0.00077	-0.00063	0.01781

This journal is © The Royal Society of Chemistry 2014

D36	0.01774	0.00001	0.00139	-0.00320	-0.00180	0.01594
D37	-3.11265	0.00002	0.00176	-0.00413	-0.00237	-3.11502
D38	-3.13443	0.00002	-0.00246	0.00719	0.00474	-3.12969
D39	0.01837	0.00003	-0.00209	0.00625	0.00416	0.02253
D40	-0.08421	0.00003	0.00432	-0.00969	-0.00538	-0.08959
D41	-2.21125	-0.00001	0.00361	-0.00844	-0.00483	-2.21608
D42	2.02374	0.00017	-0.00022	0.00325	0.00301	2.02675
D43	2.03774	-0.00004	0.00494	-0.01147	-0.00654	2.03120
D44	-0.08930	-0.00007	0.00423	-0.01022	-0.00599	-0.09529
D45	-2.13750	0.00010	0.00040	0.00147	0.00185	-2.13564
D46	-2.19422	-0.00015	0.00669	-0.01684	-0.01013	-2.20435
D47	1.96193	-0.00018	0.00599	-0.01559	-0.00959	1.95234
D48	-0.08627	-0.00001	0.00216	-0.00390	-0.00174	-0.08801
D49	-2.03755	0.00049	0.00381	0.01617	0.01995	-2.01761
D50	1.13033	-0.00072	-0.01460	-0.01472	-0.02935	1.10097
D51	2.14914	0.00055	0.00348	0.01787	0.02134	2.17048
D52	-0.96616	-0.00067	-0.01493	-0.01301	-0.02796	-0.99413
D53	0.04014	0.00049	0.00218	0.02057	0.02272	0.06286
D54	-3.07517	-0.00072	-0.01623	-0.01031	-0.02658	-3.10175
D55	-0.02436	0.00001	0.00121	-0.00194	-0.00073	-0.02509
D56	-3.11699	-0.00002	0.00358	-0.00884	-0.00526	-3.12226
D57	3.10536	0.00004	-0.00078	0.00348	0.00270	3.10806
D58	0.01273	0.00001	0.00159	-0.00341	-0.00183	0.01090
D59	-0.00201	0.00002	-0.00300	0.00787	0.00488	0.00286
D60	3.13390	0.00005	-0.00226	0.00634	0.00408	3.13798
D61	-3.13027	-0.00001	-0.00076	0.00177	0.00101	-3.12926

This journal is © The Royal Society of Chemistry 2014

D62	0.00564	0.00002	-0.00002	0.00023	0.00022	0.00586
D63	0.94800	-0.00004	-0.00102	0.00157	0.00056	0.94856
D64	-1.01153	-0.00020	-0.00124	0.00181	0.00056	-1.01097
D65	3.09532	0.00008	0.00352	-0.00892	-0.00540	3.08992
D66	-2.24704	-0.00002	-0.00360	0.00908	0.00549	-2.24155
D67	2.07662	-0.00018	-0.00382	0.00932	0.00549	2.08210
D68	-0.09972	0.00009	0.00094	-0.00142	-0.00048	-0.10019
D69	3.10266	0.00000	-0.00075	0.00200	0.00125	3.10391
D70	-0.02279	-0.00003	-0.00214	0.00447	0.00232	-0.02046
D71	0.01781	-0.00002	0.00199	-0.00598	-0.00399	0.01382
D72	-3.10763	-0.00005	0.00060	-0.00351	-0.00291	-3.11055
D73	-0.93597	-0.00003	-0.00352	0.00792	0.00440	-0.93158
D74	1.24234	0.00006	-0.00072	0.00146	0.00074	1.24308
D75	-2.95252	-0.00019	-0.00233	0.00321	0.00088	-2.95164
D76	1.04224	0.00007	-0.00195	0.00456	0.00262	1.04486
D77	-3.06263	0.00015	0.00085	-0.00190	-0.00104	-3.06367
D78	-0.97430	-0.00010	-0.00076	-0.00015	-0.00090	-0.97520
D79	-3.02220	-0.00005	-0.00334	0.00704	0.00369	-3.01851
D80	-0.84389	0.00004	-0.00055	0.00058	0.00004	-0.84385
D81	1.24444	-0.00021	-0.00215	0.00233	0.00018	1.24462
D82	1.63725	-0.00032	-0.00663	-0.01946	-0.02608	1.61117
D83	-1.44112	0.00027	0.00072	0.02700	0.02771	-1.41341
D84	-0.48307	-0.00044	-0.01119	-0.00902	-0.02019	-0.50326
D85	2.72175	0.00015	-0.00384	0.03745	0.03360	2.75534
D86	-2.60614	-0.00025	-0.00831	-0.01496	-0.02326	-2.62940
D87	0.59867	0.00034	-0.00096	0.03150	0.03053	0.62920

This journal is © The Royal Society of Chemistry 2014

D88	0.10872	-0.00050	-0.00589	-0.01384	-0.01969	0.08903
D89	-3.06685	0.00079	0.01492	0.02345	0.03846	-3.02839
D90	2.19087	-0.00046	-0.00678	-0.01069	-0.01745	2.17342
D91	-0.98470	0.00083	0.01403	0.02660	0.04070	-0.94400
D92	-2.00200	-0.00056	-0.01010	-0.00312	-0.01321	-2.01522
D93	1.10561	0.00073	0.01072	0.03417	0.04494	1.15055
D94	-0.01379	-0.00003	-0.00097	0.00185	0.00088	-0.01291
D95	3.13839	-0.00002	-0.00104	0.00237	0.00133	3.13972
D96	3.12210	0.00000	-0.00023	0.00032	0.00008	3.12218
D97	-0.00890	0.00001	-0.00030	0.00083	0.00053	-0.00836
D98	-3.13863	0.00003	0.00181	-0.00389	-0.00208	-3.14071
D99	0.01476	0.00003	0.00117	-0.00242	-0.00125	0.01351
D100	0.01877	-0.00001	0.00046	-0.00150	-0.00105	0.01772
D101	-3.11102	-0.00001	-0.00019	-0.00003	-0.00022	-3.11124
D102	0.00364	0.00000	0.00040	-0.00076	-0.00036	0.00327
D103	3.13462	0.00000	0.00047	-0.00128	-0.00082	3.13380
D104	-3.12609	0.00000	-0.00024	0.00072	0.00047	-3.12562
D105	0.00489	-0.00001	-0.00018	0.00020	0.00002	0.00491
D106	-3.13248	-0.00001	-0.00034	0.00063	0.00029	-3.13219
D107	0.01360	0.00000	0.00062	-0.00156	-0.00094	0.01266
D108	0.00623	-0.00001	0.00035	-0.00102	-0.00066	0.00556
D109	-3.13087	0.00001	0.00131	-0.00320	-0.00190	-3.13277
D110	3.13314	-0.00001	-0.00070	0.00165	0.00094	3.13408
D111	-0.00365	0.00000	-0.00085	0.00213	0.00128	-0.00236
D112	-0.00395	0.00000	0.00026	-0.00055	-0.00029	-0.00424
D113	-3.14073	0.00001	0.00012	-0.00007	0.00005	-3.14069

```
   D114       -0.01208  -0.00001  -0.00017   0.00026   0.00010  -
0.01198
   D115        3.11849  -0.00001  -0.00054   0.00122   0.00068
3.11917
   D116        3.13429   0.00000  -0.00031   0.00074   0.00043
3.13473
   D117       -0.01833  -0.00001  -0.00068   0.00170   0.00102  -
0.01731
   D118        0.02973  -0.00085  -0.00626  -0.03084  -0.03705  -
0.00732
   D119       -3.13603   0.00026   0.01069  -0.00235   0.00823  -
3.12780
   D120       -0.08929   0.00085   0.00777   0.02812   0.03584  -
0.05345
   D121        3.08310  -0.00031  -0.01112  -0.00589  -0.01679
3.06632
         Item               Value     Threshold  Converged?
 Maximum Force            0.000853     0.000450     NO
 RMS     Force            0.000212     0.000300     YES
 Maximum Displacement     0.058031     0.001800     NO
 RMS     Displacement     0.008465     0.001200     NO
 Predicted change in Energy=-1.631578D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.616194   -1.031391   -0.395588
      2          6           0       -0.181433   -1.433736   -0.668998
      3          1           0       -0.091989   -2.443633   -1.077110
      4          6           0       -1.745039    0.267284    0.130187
      5          6           0        0.338950   -0.371454   -1.706685
      6          1           0       -0.255458   -0.455230   -2.621670
      7          6           0        0.598306   -1.253771    0.621378
      8          6           0        0.480730    0.031584    1.187395
      9          6           0       -0.387647    0.975868    0.345922
     10          6           0        0.289230    1.036902   -1.079841
     11          1           0       -0.253255    1.764008   -1.692083
     12          6           0        1.385251   -2.228214    1.234375
     13          1           0        1.480097   -3.214429    0.785097
     14          6           0        1.168166    0.336148    2.364772
     15          1           0        1.123343    1.328369    2.803715
     16          6           0        1.949361   -0.649132    2.985199
     17          1           0        2.482650   -0.410030    3.901647
     18          6           0        2.057098   -1.925138    2.426041
     19          1           0        2.670438   -2.681364    2.909074
     20          6           0       -2.745895   -1.807938   -0.647040
     21          1           0       -2.639114   -2.809916   -1.057992
```

This journal is © The Royal Society of Chemistry 2014

22	6	0	-4.017746	-1.290535	-0.362511
23	1	0	-4.901897	-1.895009	-0.548385
24	6	0	-4.148361	0.000458	0.155040
25	1	0	-5.134805	0.403746	0.368897
26	6	0	-3.012765	0.788262	0.397105
27	1	0	-3.136103	1.797240	0.780030
28	6	0	1.799126	-0.577840	-2.074564
29	6	0	1.754776	1.467476	-1.024997
30	8	0	2.549881	0.509248	-1.649747
31	8	0	2.240971	2.441194	-0.524805
32	8	0	2.307217	-1.515930	-2.623736
33	6	0	-0.616573	2.364500	0.934313
34	1	0	-0.598242	2.438642	2.038502
35	8	0	-0.926081	3.328197	0.267881

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.514983	0.000000			
3	H	2.186802	1.092908	0.000000		
4	C	1.406981	2.444796	3.396941	0.000000	
5	C	2.444806	1.573542	2.208166	2.850455	0.000000
6	H	2.671891	2.185379	2.523119	3.211478	1.094320
7	C	2.446974	1.518371	2.185667	2.836572	2.503123
8	C	2.834227	2.455977	3.403335	2.475337	2.925447
9	C	2.467438	2.622743	3.715565	1.546334	2.560550
10	C	2.894249	2.548406	3.501351	2.488922	1.542359
11	H	3.369385	3.358188	4.255401	2.790388	2.216105
12	C	3.619094	2.590082	2.751656	4.152765	3.632099
13	H	3.968210	2.836537	2.556051	4.790901	3.948886
14	C	4.152398	3.762668	4.600188	3.672176	4.214862
15	H	4.827947	4.625084	5.546696	4.062176	4.883480
16	C	4.928390	4.302214	4.887709	4.758099	4.968330
17	H	5.971000	5.388517	5.962578	5.705789	6.004192
18	C	4.717356	3.851203	4.142400	4.953171	4.737656
19	H	5.658482	4.742610	4.855634	5.992760	5.663634
20	C	1.393729	2.591713	2.762660	2.431530	3.564071
21	H	2.155991	2.843481	2.573398	3.417645	3.903302
22	C	2.415720	3.851199	4.153535	2.799062	4.651054
23	H	3.400740	4.744481	4.869883	3.886094	5.579369
24	C	2.789224	4.297961	4.893458	2.418217	4.872401
25	H	3.876168	5.384186	5.968961	3.400899	5.905164
26	C	2.426913	3.753703	4.598846	1.396350	4.123695
27	H	3.419555	4.611829	5.540813	2.167515	4.791970
28	C	3.832634	2.575032	2.837677	4.258670	1.519884
29	C	4.243104	3.506091	4.325509	3.876031	2.418869
30	O	4.615481	3.492440	4.003361	4.655432	2.380566
31	O	5.191653	4.572080	5.441440	4.587284	3.595207
32	O	4.537904	3.165618	3.001478	5.213897	2.454564
33	C	3.781527	4.145666	5.238239	2.513637	3.920885
34	H	4.359145	4.743374	5.813771	3.109921	4.775080
35	O	4.463457	4.910015	5.984875	3.171568	4.380254

This journal is © The Royal Society of Chemistry 2014

		6	7	8	9	10
6	H	0.000000				
7	C	3.447309	0.000000			
8	C	3.909979	1.409375	0.000000		
9	C	3.297289	2.453420	1.534218	0.000000	
10	C	2.213680	2.869993	2.487508	1.579459	0.000000
11	H	2.406066	3.896697	3.439683	2.189221	1.094446
12	C	4.550218	1.394485	2.434554	3.768111	4.149439
13	H	4.715017	2.156046	3.420114	4.608679	4.792700
14	C	5.245720	2.427346	1.396977	2.627841	3.623388
15	H	5.875127	3.421361	2.169584	2.906560	3.982801
16	C	6.027919	2.789012	2.419164	3.881754	4.703541
17	H	7.074810	3.875928	3.401452	4.775196	5.632045
18	C	5.743512	2.415702	2.801418	4.326604	4.918358
19	H	6.641210	3.400780	3.888328	5.412668	5.950387
20	C	3.454165	3.619346	4.142476	3.781122	4.182394
21	H	3.697493	3.965193	4.780096	4.623012	4.834634
22	C	4.467252	4.719886	4.938268	4.337750	4.947885
23	H	5.287804	5.659661	5.974728	5.424037	5.985512
24	C	4.803380	4.931674	4.742912	3.889837	4.721373
25	H	5.786998	5.973246	5.687062	4.781565	5.649768
26	C	4.273407	4.154519	3.660823	2.632311	3.625791
27	H	4.994326	4.824899	4.045364	2.901226	3.971164
28	C	2.129713	3.027698	3.570706	3.613134	2.424181
29	C	3.207367	3.384253	2.929105	2.590574	1.528472
30	O	3.121663	3.474895	3.543857	3.581829	2.390346
31	O	4.360994	4.202957	3.440391	3.132886	2.467669
32	O	2.773516	3.676938	4.500619	4.721252	3.601782
33	C	4.552614	3.829588	2.590486	1.525421	2.576784
34	H	5.496289	4.132055	2.771730	2.246972	3.532216
35	O	4.807655	4.841812	3.700308	2.414426	2.922904

		11	12	13	14	15
11	H	0.000000				
12	C	5.214087	0.000000			
13	H	5.824583	1.087872	0.000000		
14	C	4.529601	2.810850	3.898624	0.000000	
15	H	4.721970	3.896243	4.983885	1.085902	0.000000
16	C	5.705412	2.424274	3.411950	1.402132	2.150757
17	H	6.595562	3.409460	4.310760	2.155606	2.464793
18	C	5.992201	1.401178	2.165156	2.430508	3.405854
19	H	7.034200	2.159089	2.492458	3.414450	4.299136
20	C	4.479304	4.558808	4.678487	5.384050	6.059302
21	H	5.197613	4.667852	4.530839	6.009028	6.796637
22	C	5.026866	5.711538	5.936720	6.080942	6.581371
23	H	6.025473	6.543508	6.651984	7.092970	7.611194
24	C	4.657663	6.062409	6.512450	5.767241	6.047288
25	H	5.470601	7.084306	7.551247	6.611772	6.778472
26	C	3.596064	5.398397	6.029749	4.642876	4.815691
27	H	3.797796	6.070697	6.813674	4.813827	4.738990
28	C	3.137326	3.720767	3.902696	4.576154	5.280901
29	C	2.136615	4.347349	5.027139	3.621401	3.882923
30	O	3.071447	4.143456	4.575880	4.249172	4.747557

31	O	2.835892	5.062642	5.854984	3.732529	3.683274
32	O	4.264035	4.030185	3.897328	5.441768	6.240899
33	C	2.718556	5.019000	5.961772	3.057076	2.756000
34	H	3.806758	5.134239	6.152050	2.765344	2.186804
35	O	2.596312	6.095086	6.990218	4.211315	3.824906
		16	17	18	19	20
16	C	0.000000				
17	H	1.086942	0.000000			
18	C	1.397303	2.157327	0.000000		
19	H	2.157711	2.485845	1.086916	0.000000	
20	C	6.048258	7.069823	5.703184	6.538003	0.000000
21	H	6.486177	7.522629	5.914028	6.629139	1.088230
22	C	6.872040	7.823904	6.714348	7.574264	1.402236
23	H	7.808852	8.748685	7.568074	8.361378	2.160014
24	C	6.753813	7.627311	6.882811	7.827700	2.424982
25	H	7.624893	8.436123	7.834476	8.768821	3.410361
26	C	5.778151	6.627013	6.097756	7.116677	2.810998
27	H	6.058833	6.796096	6.598090	7.635879	3.896935
28	C	5.062495	6.017513	4.705019	5.479110	4.920182
29	C	4.538675	5.322279	4.848803	5.790357	5.579179
30	O	4.815101	5.627395	4.772957	5.565734	5.866858
31	O	4.685646	5.270802	5.273153	6.181955	6.552778
32	O	5.686788	6.620757	5.072500	5.665876	5.433833
33	C	4.457816	5.109625	5.270176	6.337576	4.944080
34	H	4.113498	4.591093	5.122850	6.136500	5.464246
35	O	5.609914	6.228808	6.415180	7.485030	5.525277
		21	22	23	24	25
21	H	0.000000				
22	C	2.166296	0.000000			
23	H	2.493379	1.087043	0.000000		
24	C	3.412839	1.396990	2.157642	0.000000	
25	H	4.311856	2.157166	2.485946	1.086944	0.000000
26	C	3.899206	2.430720	3.415072	1.403143	2.156780
27	H	4.985099	3.408379	4.302955	2.154926	2.470964
28	C	5.070854	6.105330	6.997705	6.377944	7.417103
29	C	6.132165	6.431759	7.472936	6.196100	7.109204
30	O	6.188110	6.930362	7.907114	6.955758	7.946096
31	O	7.188440	7.288599	8.356062	6.873350	7.704022
32	O	5.347162	6.720795	7.511465	7.189959	8.247708
33	C	5.902079	5.158392	6.221400	4.320821	4.957688
34	H	6.426569	5.600413	6.632795	4.700587	5.244882
35	O	6.509136	5.593610	6.614778	4.633538	5.126009
		26	27	28	29	30
26	C	0.000000				
27	H	1.086223	0.000000			
28	C	5.579397	6.176261	0.000000		
29	C	5.021270	5.223750	2.299321	0.000000	
30	O	5.933842	6.316103	1.387755	1.393092	0.000000
31	O	5.584249	5.570475	3.422214	1.197791	2.256842
32	O	6.537353	7.224434	1.199900	3.429559	2.260285
33	C	2.918022	2.587203	4.852454	3.204192	4.488402
34	H	3.353783	2.904460	5.635943	3.983075	5.218852

This journal is © The Royal Society of Chemistry 2014

```
   35  O    3.289714   2.736846   5.307629   3.510100   4.868889
                 31         32         33         34         35
   31  O    0.000000
   32  O    4.479814   0.000000
   33  C    3.209433   6.022126   0.000000
   34  H    3.825137   6.768810   1.106827   0.000000
   35  O    3.383096   6.502401   1.211874   2.008454   0.000000
Stoichiometry    C19H12O4
Framework group  C1[X(C19H12O4)]
Deg. of freedom    99
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.612927   -1.030740   -0.413275
     2          6           0       -0.174914   -1.434028   -0.667541
     3          1           0       -0.080734   -2.443789   -1.074923
     4          6           0       -1.747874    0.267770    0.111375
     5          6           0        0.360188   -0.371623   -1.697587
     6          1           0       -0.221905   -0.454497   -2.620536
     7          6           0        0.587509   -1.255290    0.633310
     8          6           0        0.463279    0.029872    1.198344
     9          6           0       -0.392983    0.975226    0.345731
    10          6           0        0.303080    1.036460   -1.070757
    11          1           0       -0.230569    1.764277   -1.689880
    12          6           0        1.365401   -2.230629    1.256357
    13          1           0        1.465554   -3.216691    0.807897
    14          6           0        1.135022    0.333335    2.385026
    15          1           0        1.085031    1.325371    2.823828
    16          6           0        1.907056   -0.652841    3.015419
    17          1           0        2.428132   -0.414595    3.939087
    18          6           0        2.021363   -1.928649    2.457116
    19          1           0        2.627578   -2.685577    2.947982
    20          6           0       -2.739718   -1.806312   -0.680312
    21          1           0       -2.628158   -2.808167   -1.090296
    22          6           0       -4.014899   -1.288095   -0.412675
    23          1           0       -4.896917   -1.891812   -0.610746
    24          6           0       -4.151511    0.002738    0.103724
    25          1           0       -5.140445    0.406662    0.304480
    26          6           0       -3.018691    0.789568    0.361459
    27          1           0       -3.146424    1.798449    0.743200
    28          6           0        1.825033   -0.578923   -2.045872
    29          6           0        1.768075    1.465905   -0.995962
    30          8           0        2.570808    0.507389   -1.610432
    31          8           0        2.248214    2.439008   -0.488773
    32          8           0        2.339774   -1.517122   -2.588627
    33          6           0       -0.628778    2.363737    0.931689
    34          1           0       -0.625265    2.437317    2.036062
```

```
    35          8           0       -0.928564    3.327997    0.261637
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3733984      0.2662950
0.2545518
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1925.7762292434 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1032.18940842     A.U. after   15 cycles
             Convg  =    0.2773D-08             -V/T =  2.0094
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.001132646    0.000222619    0.000170191
      2        6           0.000303063    0.000184352   -0.000182446
      3        1           0.000170563    0.000225158   -0.000114620
      4        6          -0.001238634    0.000093727    0.000071253
      5        6           0.000072149   -0.000015915   -0.000891178
      6        1          -0.000252624    0.000011469    0.000338596
      7        6           0.000719313   -0.000007555    0.000549031
      8        6           0.000503891   -0.000381823    0.000288260
      9        6           0.001830810    0.000549552   -0.000382457
     10        6          -0.000411811    0.000451288   -0.000147077
     11        1          -0.000407076   -0.000096812    0.000293713
     12        6           0.000069735    0.000768367    0.000346836
     13        1          -0.000068092    0.000270250    0.000121445
     14        6           0.000364299   -0.000715637   -0.000461628
```

15	1	-0.000045452	-0.000152928	-0.000152670
16	6	-0.000483912	-0.000337413	-0.000972155
17	1	-0.000191224	-0.000061160	-0.000190126
18	6	-0.000600141	0.000774894	-0.000476287
19	1	-0.000171906	0.000151784	-0.000115950
20	6	-0.000298540	0.000846460	0.000392561
21	1	0.000021749	0.000319588	0.000088160
22	6	0.000970355	0.000536278	0.000239159
23	1	0.000222326	0.000116804	0.000012277
24	6	0.001165243	-0.000439460	-0.000315412
25	1	0.000261225	-0.000049898	-0.000013825
26	6	-0.000095563	-0.000741503	-0.000374158
27	1	0.000159716	-0.000264150	-0.000202659
28	6	0.001375545	-0.001648749	0.002006182
29	6	0.000716000	-0.001194097	0.003745369
30	8	-0.000798826	0.000612356	-0.001434569
31	8	-0.001288668	-0.000096000	-0.001309638
32	8	-0.001056753	0.001361862	-0.000107795
33	6	-0.004078781	-0.000454210	-0.000578167
34	1	0.001642224	-0.000314352	0.000408086
35	8	0.002052441	-0.000525147	-0.000648303

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.004078781 RMS     0.000863550


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.002462507 RMS     0.000487397
 Search for a local minimum.
 Step number   3 out of a maximum of  210
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3
 DE=  1.03D-04 DEPred=-1.63D-04 R=-6.32D-01
 Trust test=-6.32D-01 RLast= 1.37D-01 DXMaxT set to 1.50D-01
     Eigenvalues ---    0.00417   0.00459   0.00625   0.00773
0.01067
     Eigenvalues ---    0.01149   0.01172   0.01430   0.01476
0.01569
     Eigenvalues ---    0.01801   0.02115   0.02121   0.02128
0.02131
     Eigenvalues ---    0.02133   0.02135   0.02142   0.02144
0.02150
     Eigenvalues ---    0.02156   0.02160   0.02165   0.02755
0.03402
     Eigenvalues ---    0.03783   0.04168   0.04691   0.05199
0.05280
     Eigenvalues ---    0.05352   0.05740   0.06330   0.06622
0.08141
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.08562   0.09339   0.09930   0.12460
0.15542
     Eigenvalues ---    0.15998   0.15999   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16026   0.16405
0.20180
     Eigenvalues ---    0.21651   0.21997   0.22000   0.22171
0.22607
     Eigenvalues ---    0.22636   0.22732   0.24235   0.24571
0.24630
     Eigenvalues ---    0.24801   0.25001   0.26714   0.27077
0.27653
     Eigenvalues ---    0.28814   0.28841   0.29726   0.29956
0.31044
     Eigenvalues ---    0.32535   0.34345   0.34405   0.34527
0.35124
     Eigenvalues ---    0.35161   0.35233   0.35244   0.35248
0.35267
     Eigenvalues ---    0.35346   0.35370   0.36714   0.39994
0.42010
     Eigenvalues ---    0.42045   0.43150   0.43937   0.44323
0.45477
     Eigenvalues ---    0.46050   0.46171   0.46324   0.46409
0.46798
     Eigenvalues ---    0.47039   0.97756   1.04177
1.066811000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     3    2    1
 RFO step:  Lambda=-1.28131412D-04.
 DIIS coeffs:      0.31712      0.44238      0.24050
 Iteration  1 RMS(Cart)=  0.00973444 RMS(Int)=  0.00029036
 Iteration  2 RMS(Cart)=  0.00027294 RMS(Int)=  0.00013779
 Iteration  3 RMS(Cart)=  0.00000018 RMS(Int)=  0.00013779
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86290   0.00009   0.00039   0.00023   0.00063
2.86354
    R2        2.65881  -0.00074  -0.00109   0.00046  -0.00063
2.65817
    R3        2.63377  -0.00134  -0.00215   0.00111  -0.00104
2.63273
    R4        2.06530  -0.00015  -0.00035   0.00020  -0.00015
2.06515
    R5        2.97356  -0.00094  -0.00143   0.00028  -0.00116
2.97241
    R6        2.86931  -0.00035  -0.00021  -0.00048  -0.00069
2.86862
    R7        2.92215  -0.00017  -0.00209   0.00140  -0.00070
2.92145
    R8        2.63872  -0.00145  -0.00254   0.00136  -0.00118
2.63753
```

This journal is © The Royal Society of Chemistry 2014

R9	2.06797	-0.00015	-0.00053	0.00032	-0.00021
2.06775					
R10	2.91464	-0.00067	-0.00263	0.00203	-0.00061
2.91402					
R11	2.87216	-0.00036	0.00088	-0.00114	-0.00025
2.87192					
R12	2.66333	-0.00092	-0.00113	0.00034	-0.00078
2.66255					
R13	2.63519	-0.00126	-0.00215	0.00115	-0.00100
2.63419					
R14	2.89925	-0.00051	-0.00195	0.00154	-0.00041
2.89884					
R15	2.63990	-0.00131	-0.00205	0.00106	-0.00099
2.63891					
R16	2.98474	-0.00246	-0.00476	0.00101	-0.00376
2.98099					
R17	2.88263	-0.00144	-0.00151	-0.00029	-0.00180
2.88083					
R18	2.06820	-0.00003	-0.00081	0.00072	-0.00009
2.06812					
R19	2.88839	-0.00118	-0.00174	0.00019	-0.00157
2.88683					
R20	2.05578	-0.00030	-0.00073	0.00041	-0.00032
2.05546					
R21	2.64784	-0.00131	-0.00228	0.00120	-0.00108
2.64676					
R22	2.05206	-0.00020	-0.00043	0.00020	-0.00023
2.05183					
R23	2.64965	-0.00122	-0.00226	0.00128	-0.00099
2.64866					
R24	2.05402	-0.00027	-0.00054	0.00025	-0.00029
2.05374					
R25	2.64052	-0.00123	-0.00240	0.00139	-0.00101
2.63951					
R26	2.05397	-0.00026	-0.00051	0.00024	-0.00027
2.05370					
R27	2.05646	-0.00032	-0.00071	0.00036	-0.00034
2.05611					
R28	2.64984	-0.00144	-0.00255	0.00140	-0.00115
2.64869					
R29	2.05421	-0.00025	-0.00050	0.00024	-0.00026
2.05395					
R30	2.63993	-0.00118	-0.00219	0.00123	-0.00096
2.63897					
R31	2.05403	-0.00026	-0.00050	0.00022	-0.00028
2.05375					
R32	2.65156	-0.00137	-0.00262	0.00147	-0.00115
2.65040					
R33	2.05266	-0.00034	-0.00054	0.00021	-0.00033
2.05234					
R34	2.62248	-0.00016	0.00003	-0.00015	-0.00011
2.62237					

This journal is © The Royal Society of Chemistry 2014

R35	2.26748	-0.00146	-0.00217	0.00166	-0.00052	2.26696
R36	2.63256	-0.00010	-0.00160	0.00143	-0.00018	2.63239
R37	2.26350	-0.00115	-0.00128	0.00086	-0.00042	2.26308
R38	2.09160	0.00041	0.00185	-0.00144	0.00041	2.09201
R39	2.29011	-0.00058	-0.00170	0.00145	-0.00025	2.28986
A1	1.98155	-0.00008	-0.00032	0.00060	0.00028	1.98183
A2	2.19828	0.00008	0.00090	-0.00101	-0.00010	2.19817
A3	2.10305	0.00000	-0.00065	0.00046	-0.00019	2.10286
A4	1.97176	0.00016	0.00159	-0.00087	0.00072	1.97248
A5	1.82649	-0.00011	0.00142	-0.00065	0.00076	1.82725
A6	1.87706	0.00014	0.00111	-0.00051	0.00060	1.87765
A7	1.92889	0.00010	-0.00161	0.00095	-0.00066	1.92823
A8	1.96583	0.00000	0.00019	-0.00010	0.00010	1.96594
A9	1.88661	-0.00031	-0.00277	0.00121	-0.00156	1.88505
A10	1.97655	-0.00008	-0.00033	-0.00035	-0.00068	1.97587
A11	2.09319	0.00004	0.00069	-0.00036	0.00034	2.09353
A12	2.21344	0.00004	-0.00041	0.00072	0.00033	2.21377
A13	1.89660	0.00010	0.00102	-0.00136	-0.00034	1.89627
A14	1.91533	-0.00009	-0.00061	0.00018	-0.00042	1.91491
A15	1.96672	-0.00021	-0.00332	0.00317	-0.00015	1.96657
A16	1.97383	-0.00012	0.00034	-0.00006	0.00028	1.97411
A17	1.88500	0.00035	0.00283	-0.00157	0.00126	1.88626
A18	1.82692	-0.00003	-0.00038	-0.00023	-0.00060	1.82633
A19	1.98948	-0.00003	-0.00051	0.00020	-0.00031	1.98917
A20	2.19021	0.00000	0.00062	-0.00053	0.00010	2.19031
A21	2.10346	0.00003	-0.00015	0.00036	0.00021	2.10367

This journal is © The Royal Society of Chemistry 2014

A22	1.96955	0.00005	-0.00006	0.00019	0.00013
1.96968					
A23	2.09008	0.00002	0.00012	-0.00024	-0.00011
2.08996					
A24	2.22256	-0.00008	-0.00026	0.00018	-0.00007
2.22249					
A25	1.86641	0.00020	0.00213	-0.00052	0.00162
1.86803					
A26	1.84207	0.00003	-0.00061	0.00004	-0.00058
1.84149					
A27	1.91688	0.00016	0.00253	-0.00083	0.00173
1.91861					
A28	1.85076	-0.00005	-0.00026	-0.00007	-0.00034
1.85042					
A29	2.01936	0.00020	0.00212	-0.00162	0.00053
2.01989					
A30	1.95770	-0.00052	-0.00594	0.00301	-0.00294
1.95477					
A31	1.92346	0.00033	0.00133	-0.00052	0.00083
1.92429					
A32	1.97715	-0.00007	0.00359	-0.00269	0.00090
1.97805					
A33	1.81409	0.00028	0.00067	0.00027	0.00094
1.81503					
A34	1.89465	-0.00004	-0.00214	0.00176	-0.00038
1.89428					
A35	1.97078	-0.00085	-0.00771	0.00432	-0.00339
1.96739					
A36	1.88408	0.00032	0.00424	-0.00322	0.00105
1.88513					
A37	2.09571	0.00003	-0.00019	0.00025	0.00005
2.09577					
A38	2.08667	-0.00010	-0.00026	0.00006	-0.00020
2.08647					
A39	2.10078	0.00008	0.00046	-0.00031	0.00015
2.10093					
A40	2.11715	-0.00003	-0.00079	0.00073	-0.00006
2.11709					
A41	2.08736	-0.00013	-0.00038	0.00022	-0.00016
2.08721					
A42	2.07855	0.00016	0.00119	-0.00095	0.00023
2.07878					
A43	2.08502	-0.00008	-0.00011	-0.00002	-0.00014
2.08488					
A44	2.10318	0.00011	0.00023	-0.00005	0.00018
2.10336					
A45	2.09492	-0.00003	-0.00011	0.00007	-0.00004
2.09488					
A46	2.09542	0.00007	0.00039	-0.00035	0.00004
2.09546					
A47	2.09213	-0.00005	-0.00025	0.00019	-0.00007
2.09206					

A48	2.09558	-0.00001	-0.00013	0.00016	0.00003	2.09561
A49	2.09625	-0.00001	-0.00029	0.00020	-0.00008	2.09617
A50	2.08633	-0.00010	-0.00017	0.00006	-0.00011	2.08622
A51	2.10060	0.00011	0.00046	-0.00027	0.00019	2.10079
A52	2.09191	-0.00007	-0.00033	0.00018	-0.00015	2.09176
A53	2.09551	0.00006	0.00047	-0.00036	0.00011	2.09562
A54	2.09576	0.00001	-0.00015	0.00019	0.00004	2.09580
A55	2.09511	-0.00003	-0.00011	0.00015	0.00004	2.09515
A56	2.10261	0.00017	0.00016	0.00003	0.00020	2.10281
A57	2.08545	-0.00015	-0.00005	-0.00018	-0.00024	2.08521
A58	2.08554	-0.00017	-0.00054	0.00017	-0.00037	2.08517
A59	2.11419	-0.00005	-0.00158	0.00146	-0.00011	2.11408
A60	2.08340	0.00021	0.00211	-0.00163	0.00048	2.08389
A61	1.91694	-0.00016	-0.00023	0.00023	0.00018	1.91711
A62	2.24433	-0.00029	-0.00150	0.00073	-0.00063	2.24370
A63	2.12169	0.00046	0.00174	-0.00137	0.00051	2.12221
A64	1.91494	-0.00005	-0.00003	-0.00051	-0.00034	1.91460
A65	2.25646	-0.00082	-0.00293	0.00168	-0.00102	2.25544
A66	2.11154	0.00089	0.00289	-0.00165	0.00147	2.11301
A67	1.94694	-0.00008	-0.00072	0.00063	-0.00008	1.94685
A68	2.03007	-0.00014	-0.00204	0.00480	0.00159	2.03166
A69	2.15330	-0.00081	-0.00140	0.00211	-0.00046	2.15284
A70	2.09390	0.00116	0.00605	-0.00024	0.00464	2.09854
D1	-3.14150	0.00011	0.00110	-0.00016	0.00093	-3.14056
D2	-1.04213	0.00025	0.00093	0.00009	0.00102	-1.04111
D3	0.96141	-0.00010	-0.00107	0.00094	-0.00013	0.96127

This journal is © The Royal Society of Chemistry 2014

D4	-0.02676	0.00005	-0.00194	0.00210	0.00016	-0.02660
D5	2.07262	0.00019	-0.00211	0.00236	0.00024	2.07286
D6	-2.20703	-0.00015	-0.00411	0.00320	-0.00091	-2.20794
D7	-0.02739	0.00000	0.00047	-0.00075	-0.00028	-0.02767
D8	3.11068	-0.00011	-0.00513	0.00284	-0.00229	3.10839
D9	3.13942	0.00005	0.00330	-0.00285	0.00045	3.13987
D10	-0.00569	-0.00005	-0.00231	0.00074	-0.00156	-0.00725
D11	0.02373	0.00004	0.00307	-0.00240	0.00066	0.02439
D12	-3.12169	0.00006	0.00407	-0.00277	0.00130	-3.12039
D13	3.13675	-0.00002	-0.00016	0.00001	-0.00016	3.13660
D14	-0.00867	0.00000	0.00084	-0.00036	0.00048	-0.00819
D15	-1.08972	-0.00003	-0.00537	0.00218	-0.00319	-1.09291
D16	1.07676	-0.00018	-0.00466	0.00132	-0.00334	1.07342
D17	3.10507	-0.00040	-0.00752	0.00307	-0.00444	3.10062
D18	1.03800	0.00014	-0.00348	0.00125	-0.00223	1.03578
D19	-3.07871	0.00000	-0.00278	0.00040	-0.00238	-3.08108
D20	-1.05040	-0.00023	-0.00563	0.00215	-0.00348	-1.05388
D21	-3.08654	0.00000	-0.00610	0.00254	-0.00356	-3.09010
D22	-0.92007	-0.00015	-0.00539	0.00169	-0.00371	-0.92378
D23	1.10824	-0.00037	-0.00825	0.00344	-0.00481	1.10343
D24	-0.93645	0.00006	0.00028	-0.00041	-0.00013	-0.93658
D25	2.21407	0.00013	0.00384	-0.00292	0.00092	2.21499
D26	-3.12028	-0.00024	-0.00271	0.00115	-0.00156	-3.12184
D27	0.03024	-0.00017	0.00085	-0.00136	-0.00051	0.02973
D28	1.02673	-0.00014	0.00113	-0.00084	0.00029	1.02702
D29	-2.10594	-0.00007	0.00469	-0.00335	0.00135	-2.10459

This journal is © The Royal Society of Chemistry 2014

D30	-0.92359	0.00008	0.00018	0.00083	0.00101	-0.92258
D31	1.04189	0.00012	0.00052	0.00054	0.00107	1.04295
D32	-3.12760	-0.00040	-0.00556	0.00371	-0.00184	-3.12944
D33	2.22181	0.00020	0.00624	-0.00306	0.00319	2.22500
D34	-2.09589	0.00024	0.00658	-0.00334	0.00324	-2.09265
D35	0.01781	-0.00028	0.00050	-0.00017	0.00033	0.01814
D36	0.01594	0.00006	0.00194	-0.00047	0.00147	0.01741
D37	-3.11502	0.00010	0.00252	-0.00069	0.00183	-3.11319
D38	-3.12969	-0.00006	-0.00449	0.00365	-0.00084	-3.13053
D39	0.02253	-0.00003	-0.00391	0.00343	-0.00048	0.02205
D40	-0.08959	0.00017	0.00588	-0.00188	0.00399	-0.08560
D41	-2.21608	0.00002	0.00514	-0.00190	0.00324	-2.21284
D42	2.02675	-0.00049	-0.00217	0.00312	0.00096	2.02771
D43	2.03120	0.00015	0.00699	-0.00353	0.00345	2.03465
D44	-0.09529	0.00000	0.00625	-0.00356	0.00269	-0.09259
D45	-2.13564	-0.00052	-0.00106	0.00147	0.00041	-2.13523
D46	-2.20435	0.00049	0.01034	-0.00559	0.00474	-2.19962
D47	1.95234	0.00034	0.00960	-0.00562	0.00398	1.95633
D48	-0.08801	-0.00018	0.00229	-0.00059	0.00170	-0.08631
D49	-2.01761	-0.00001	-0.01167	0.00919	-0.00247	-2.02008
D50	1.10097	0.00066	0.01258	-0.01189	0.00071	1.10168
D51	2.17048	-0.00023	-0.01279	0.00998	-0.00281	2.16767
D52	-0.99413	0.00043	0.01147	-0.01110	0.00038	-0.99375
D53	0.06286	-0.00025	-0.01440	0.01095	-0.00344	0.05942
D54	-3.10175	0.00041	0.00986	-0.01013	-0.00025	-3.10200
D55	-0.02509	0.00001	0.00112	0.00021	0.00133	-0.02376

This journal is © The Royal Society of Chemistry 2014

D56	-3.12226	0.00014	0.00542	-0.00287	0.00255	-3.11971
D57	3.10806	-0.00005	-0.00224	0.00258	0.00034	3.10840
D58	0.01090	0.00007	0.00206	-0.00050	0.00155	0.01245
D59	0.00286	-0.00009	-0.00486	0.00327	-0.00159	0.00128
D60	3.13798	-0.00005	-0.00394	0.00295	-0.00099	3.13699
D61	-3.12926	-0.00001	-0.00108	0.00061	-0.00047	-3.12973
D62	0.00586	0.00003	-0.00016	0.00029	0.00013	0.00599
D63	0.94856	0.00000	-0.00090	-0.00025	-0.00115	0.94741
D64	-1.01097	-0.00010	-0.00102	-0.00004	-0.00105	-1.01202
D65	3.08992	0.00049	0.00549	-0.00280	0.00269	3.09261
D66	-2.24155	-0.00014	-0.00559	0.00311	-0.00248	-2.24403
D67	2.08210	-0.00023	-0.00570	0.00332	-0.00238	2.07973
D68	-0.10019	0.00036	0.00081	0.00056	0.00136	-0.09883
D69	3.10391	-0.00005	-0.00124	0.00057	-0.00066	3.10324
D70	-0.02046	-0.00012	-0.00268	0.00045	-0.00223	-0.02270
D71	0.01382	0.00009	0.00374	-0.00300	0.00074	0.01456
D72	-3.11055	0.00002	0.00230	-0.00312	-0.00083	-3.11138
D73	-0.93158	-0.00027	-0.00480	0.00115	-0.00364	-0.93522
D74	1.24308	-0.00016	-0.00088	-0.00136	-0.00222	1.24086
D75	-2.95164	-0.00032	-0.00179	-0.00149	-0.00328	-2.95492
D76	1.04486	-0.00005	-0.00278	0.00056	-0.00222	1.04263
D77	-3.06367	0.00005	0.00114	-0.00195	-0.00080	-3.06447
D78	-0.97520	-0.00010	0.00023	-0.00208	-0.00186	-0.97706
D79	-3.01851	-0.00019	-0.00423	0.00047	-0.00376	-3.02227
D80	-0.84385	-0.00008	-0.00030	-0.00204	-0.00234	-0.84619
D81	1.24462	-0.00024	-0.00122	-0.00217	-0.00339	1.24122

This journal is © The Royal Society of Chemistry 2014

D82	1.61117	0.00117	0.01442	0.02629	0.04071	1.65189
D83	-1.41341	-0.00097	-0.01855	-0.03944	-0.05801	-1.47142
D84	-0.50326	0.00064	0.00807	0.02877	0.03685	-0.46640
D85	2.75534	-0.00150	-0.02490	-0.03697	-0.06187	2.69347
D86	-2.62940	0.00098	0.01164	0.02766	0.03930	-2.59009
D87	0.62920	-0.00115	-0.02134	-0.03808	-0.05942	0.56978
D88	0.08903	0.00053	0.01044	-0.00997	0.00046	0.08948
D89	-3.02839	-0.00060	-0.01863	0.01304	-0.00563	-3.03403
D90	2.17342	0.00066	0.00845	-0.00816	0.00027	2.17369
D91	-0.94400	-0.00046	-0.02063	0.01484	-0.00582	-0.94982
D92	-2.01522	0.00031	0.00387	-0.00546	-0.00158	-2.01679
D93	1.15055	-0.00081	-0.02521	0.01754	-0.00767	1.14288
D94	-0.01291	-0.00007	-0.00110	-0.00002	-0.00112	-0.01403
D95	3.13972	-0.00005	-0.00144	0.00057	-0.00087	3.13885
D96	3.12218	-0.00003	-0.00018	-0.00034	-0.00052	3.12167
D97	-0.00836	-0.00001	-0.00052	0.00025	-0.00027	-0.00863
D98	-3.14071	0.00009	0.00235	-0.00060	0.00174	-3.13897
D99	0.01351	0.00008	0.00145	-0.00019	0.00126	0.01477
D100	0.01772	0.00003	0.00095	-0.00074	0.00021	0.01793
D101	-3.11124	0.00001	0.00005	-0.00032	-0.00027	-3.11151
D102	0.00327	0.00002	0.00045	-0.00003	0.00043	0.00370
D103	3.13380	0.00000	0.00079	-0.00062	0.00017	3.13397
D104	-3.12562	0.00000	-0.00045	0.00039	-0.00005	-3.12567
D105	0.00491	-0.00001	-0.00011	-0.00020	-0.00031	0.00460
D106	-3.13219	-0.00001	-0.00037	-0.00002	-0.00039	-3.13258
D107	0.01266	0.00004	0.00096	-0.00029	0.00067	0.01333

```
   D108       0.00556   0.00001   0.00063  -0.00039   0.00025
0.00581
   D109      -3.13277   0.00007   0.00196  -0.00066   0.00131  -
3.13146
   D110       3.13408  -0.00004  -0.00100   0.00023  -0.00077
3.13331
   D111      -0.00236  -0.00004  -0.00131   0.00056  -0.00075  -
0.00311
   D112      -0.00424   0.00001   0.00033  -0.00004   0.00029  -
0.00395
   D113      -3.14069   0.00002   0.00003   0.00029   0.00032  -
3.14037
   D114      -0.01198  -0.00002  -0.00015  -0.00018  -0.00033  -
0.01231
   D115       3.11917  -0.00005  -0.00074   0.00006  -0.00068
3.11848
   D116       3.13473  -0.00001  -0.00045   0.00015  -0.00030
3.13442
   D117      -0.01731  -0.00005  -0.00104   0.00038  -0.00066  -
0.01797
   D118      -0.00732   0.00060   0.02211  -0.01820   0.00389  -
0.00343
   D119      -3.12780   0.00000  -0.00016   0.00111   0.00099  -
3.12681
   D120      -0.05345  -0.00071  -0.02050   0.01779  -0.00270  -
0.05615
   D121       3.06632   0.00028   0.00578  -0.00293   0.00277
3.06909
         Item               Value     Threshold  Converged?
 Maximum Force            0.002463     0.000450     NO
 RMS     Force            0.000487     0.000300     NO
 Maximum Displacement     0.104889     0.001800     NO
 RMS     Displacement     0.009736     0.001200     NO
 Predicted change in Energy=-2.075937D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.619287   -1.033819   -0.394857
      2          6           0       -0.183835   -1.434935   -0.668299
      3          1           0       -0.092773   -2.444121   -1.077600
      4          6           0       -1.749660    0.264220    0.131213
      5          6           0        0.337093   -0.371920   -1.704031
      6          1           0       -0.254534   -0.457267   -2.620538
      7          6           0        0.596216   -1.254869    0.621445
      8          6           0        0.477891    0.030011    1.187356
      9          6           0       -0.392912    0.973083    0.347433
```

10	6	0	0.281970	1.035796	-1.077001
11	1	0	-0.262949	1.761661	-1.688471
12	6	0	1.384729	-2.228158	1.233057
13	1	0	1.479692	-3.214232	0.783901
14	6	0	1.167759	0.335791	2.362372
15	1	0	1.122871	1.328060	2.800901
16	6	0	1.949866	-0.648622	2.981847
17	1	0	2.483879	-0.409013	3.897561
18	6	0	2.057353	-1.924388	2.423434
19	1	0	2.671454	-2.680063	2.906040
20	6	0	-2.747821	-1.810709	-0.647440
21	1	0	-2.639977	-2.812218	-1.058776
22	6	0	-4.019663	-1.294143	-0.364351
23	1	0	-4.903141	-1.898951	-0.551522
24	6	0	-4.151591	-0.003406	0.152140
25	1	0	-5.138389	0.399545	0.364243
26	6	0	-3.017371	0.784893	0.395508
27	1	0	-3.141441	1.794116	0.777054
28	6	0	1.799169	-0.574192	-2.066064
29	6	0	1.744970	1.471527	-1.018161
30	8	0	2.544749	0.516580	-1.641760
31	8	0	2.224453	2.449611	-0.520549
32	8	0	2.311245	-1.510884	-2.613319
33	6	0	-0.619899	2.361987	0.933464
34	1	0	-0.562547	2.446636	2.035775
35	8	0	-0.870576	3.336831	0.258813

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515317	0.000000			
3	H	2.187541	1.092829	0.000000		
4	C	1.406646	2.445027	3.397295	0.000000	
5	C	2.445295	1.572929	2.207083	2.850848	0.000000
6	H	2.673690	2.184507	2.520796	3.213732	1.094208
7	C	2.447486	1.518007	2.185356	2.837445	2.500917
8	C	2.834305	2.455078	3.402501	2.476343	2.922583
9	C	2.466302	2.621827	3.714578	1.545963	2.559384
10	C	2.891955	2.547258	3.500036	2.486489	1.542034
11	H	3.365679	3.356372	4.253319	2.786375	2.216407
12	C	3.619483	2.589353	2.751143	4.153360	3.629000
13	H	3.968292	2.835860	2.555563	4.791069	3.946400
14	C	4.152802	3.761282	4.598941	3.673489	4.210284
15	H	4.828122	4.623524	5.545260	4.063302	4.878708
16	C	4.928423	4.300527	4.886236	4.758769	4.963371
17	H	5.970863	5.386678	5.960959	5.706266	5.998992
18	C	4.717368	3.849845	4.141305	4.953547	4.733437
19	H	5.658311	4.741193	4.854483	5.992888	5.659462
20	C	1.393178	2.591460	2.763246	2.430629	3.564154
21	H	2.155296	2.842888	2.573732	3.416608	3.903120
22	C	2.414644	3.850426	4.153509	2.797677	4.650436
23	H	3.399514	4.743500	4.869662	3.884570	5.578544

This journal is © The Royal Society of Chemistry 2014

24	C	2.788103	4.297148	4.893194	2.416886	4.871289
25	H	3.874899	5.383221	5.968550	3.399427	5.903712
26	C	2.426320	3.753431	4.598897	1.395723	4.122949
27	H	3.418705	4.611209	5.540467	2.166736	4.790375
28	C	3.832757	2.574282	2.837805	4.257364	1.519753
29	C	4.240694	3.505740	4.325867	3.871832	2.418849
30	O	4.614942	3.493023	4.005065	4.652855	2.380558
31	O	5.188874	4.572896	5.443202	4.581953	3.594968
32	O	4.538528	3.164536	3.001443	5.212906	2.453837
33	C	3.780834	4.143962	5.236498	2.514079	3.917456
34	H	4.374727	4.745739	5.816640	3.130421	4.768623
35	O	4.482235	4.909267	5.984178	3.198438	4.366470

		6	7	8	9	10
6	H	0.000000				
7	C	3.445345	0.000000			
8	C	3.908189	1.408962	0.000000		
9	C	3.297559	2.453004	1.534000	0.000000	
10	C	2.213499	2.868905	2.485418	1.577470	0.000000
11	H	2.406753	3.895296	3.437708	2.187155	1.094400
12	C	4.546804	1.393956	2.433880	3.767265	4.147993
13	H	4.711539	2.155464	3.419283	4.607685	4.791684
14	C	5.242256	2.426455	1.396453	2.627131	3.619933
15	H	5.871681	3.420368	2.168976	2.905704	3.978776
16	C	6.023513	2.787723	2.418150	3.880551	4.700361
17	H	7.070138	3.874491	3.400285	4.773838	5.628690
18	C	5.739244	2.414610	2.800404	4.325381	4.916068
19	H	6.636662	3.399582	3.887170	5.411311	5.948265
20	C	3.455633	3.619615	4.142456	3.779532	4.179324
21	H	3.698004	3.965025	4.779589	4.621172	4.831699
22	C	4.468438	4.720135	4.938540	4.335928	4.943737
23	H	5.288556	5.659825	5.974956	5.422072	5.981157
24	C	4.804246	4.932350	4.743932	3.888359	4.716693
25	H	5.787493	5.974022	5.688292	4.780039	5.644669
26	C	4.274665	4.155681	3.662475	2.631636	3.621724
27	H	4.994655	4.826034	4.047219	2.900531	3.966398
28	C	2.130448	3.022106	3.563085	3.608912	2.423262
29	C	3.207159	3.382481	2.923656	2.585311	1.527642
30	O	3.121277	3.472306	3.537308	3.577029	2.389290
31	O	4.359503	4.204578	3.438296	3.127959	2.466121
32	O	2.773695	3.670227	4.492290	4.716843	3.600528
33	C	4.551111	3.828569	2.589926	1.524470	2.571794
34	H	5.496251	4.128463	2.764490	2.247362	3.520378
35	O	4.802640	4.833911	3.689934	2.413155	2.899573

		11	12	13	14	15
11	H	0.000000				
12	C	5.212372	0.000000			
13	H	5.823137	1.087704	0.000000		
14	C	4.526517	2.810029	3.897632	0.000000	
15	H	4.718365	3.895304	4.982773	1.085781	0.000000
16	C	5.702446	2.423341	3.410922	1.401610	2.150334
17	H	6.592469	3.408373	4.309586	2.154927	2.464230
18	C	5.989868	1.400607	2.164593	2.429715	3.405019

This journal is © The Royal Society of Chemistry 2014

19	H	7.032009	2.158414	2.491808	3.413509	4.298163
20	C	4.474389	4.559441	4.678726	5.384997	6.060130
21	H	5.192990	4.668177	4.530865	6.009415	6.796913
22	C	5.020372	5.712403	5.937014	6.082849	6.583345
23	H	6.018647	6.544494	6.652359	7.095116	7.613485
24	C	4.650252	6.063723	6.513054	5.770240	6.050511
25	H	5.462500	7.085953	7.552119	6.615443	6.782537
26	C	3.589413	5.399856	6.030541	4.646026	4.818978
27	H	3.790195	6.072301	6.814578	4.817588	4.743155
28	C	3.138648	3.713699	3.897971	4.564842	5.269088
29	C	2.136640	4.345737	5.027339	3.612627	3.872057
30	O	3.071738	4.140508	4.575711	4.238143	4.734710
31	O	2.832752	5.065747	5.859639	3.727743	3.674696
32	O	4.265133	4.020885	3.890241	5.429112	6.227809
33	C	2.713365	5.017741	5.960275	3.056627	2.755644
34	H	3.798547	5.127372	6.146818	2.748872	2.162698
35	O	2.577264	6.083146	6.979678	4.193568	3.804104

		16	17	18	19	20
16	C	0.000000				
17	H	1.086791	0.000000			
18	C	1.396766	2.156695	0.000000		
19	H	2.157124	2.485149	1.086771	0.000000	
20	C	6.049002	7.070535	5.703761	6.538465	0.000000
21	H	6.486481	7.522936	5.914299	6.629368	1.088048
22	C	6.873792	7.825817	6.715585	7.575439	1.401628
23	H	7.811000	8.751132	7.569642	8.362975	2.159257
24	C	6.756576	7.630345	6.884761	7.829584	2.424095
25	H	7.628490	8.440205	7.837068	8.771451	3.409331
26	C	5.780792	6.629746	6.099632	7.118385	2.810257
27	H	6.062136	6.799674	6.600401	7.638102	3.896008
28	C	5.050708	6.005076	4.695240	5.469679	4.921035
29	C	4.531786	5.314767	4.845039	5.787350	5.576349
30	O	4.805135	5.616450	4.766727	5.560311	5.866536
31	O	4.684146	5.268656	5.275114	6.185052	6.549040
32	O	5.672739	6.605716	5.060072	5.653321	5.435874
33	C	4.456830	5.108596	5.268842	6.336112	4.943551
34	H	4.097304	4.571837	5.110774	6.123656	5.486352
35	O	5.590496	6.206787	6.398342	7.467047	5.553603

		21	22	23	24	25
21	H	0.000000				
22	C	2.165713	0.000000			
23	H	2.492645	1.086903	0.000000		
24	C	3.411850	1.396485	2.157094	0.000000	
25	H	4.310739	2.156613	2.485367	1.086797	0.000000
26	C	3.898278	2.429890	3.414090	1.402533	2.155966
27	H	4.983980	3.407554	4.302028	2.154532	2.470434
28	C	5.072416	6.105159	6.997841	6.376344	7.415137
29	C	6.130243	6.427082	7.468283	6.189867	7.102169
30	O	6.188872	6.928347	7.905344	6.951937	7.941558
31	O	7.186042	7.282106	8.349463	6.864673	7.693963
32	O	5.350202	6.721995	7.513252	7.189471	8.246978
33	C	5.901028	5.158489	6.221490	4.321852	4.959026

This journal is © The Royal Society of Chemistry 2014

34	H	6.445736	5.630781	6.664757	4.736246	5.284215
35	O	6.532811	5.634803	6.658201	4.683335	5.181987

		26	27	28	29	30
26	C	0.000000				
27	H	1.086049	0.000000			
28	C	5.577231	6.172667	0.000000		
29	C	5.014959	5.215732	2.299131	0.000000	
30	O	5.929556	6.309953	1.387698	1.392999	0.000000
31	O	5.575586	5.559340	3.422406	1.197568	2.257502
32	O	6.535883	7.221456	1.199625	3.429281	2.260322
33	C	2.919674	2.589424	4.844606	3.192861	4.477980
34	H	3.387924	2.942933	5.614997	3.949936	5.186971
35	O	3.337635	2.793809	5.275291	3.457036	4.819797

		31	32	33	34	35
31	O	0.000000				
32	O	4.480261	0.000000			
33	C	3.195648	6.014183	0.000000		
34	H	3.781821	6.747942	1.107043	0.000000	
35	O	3.312668	6.470971	1.211740	2.011199	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.623933	-1.019979	-0.416573
2	6	0	-0.188679	-1.429148	-0.678895
3	1	0	-0.100688	-2.435395	-1.096028
4	6	0	-1.750350	0.274380	0.119437
5	6	0	0.350439	-0.361040	-1.699975
6	1	0	-0.232381	-0.434159	-2.623157
7	6	0	0.579414	-1.265911	0.620233
8	6	0	0.464542	0.014858	1.196087
9	6	0	-0.390827	0.971461	0.355605
10	6	0	0.299022	1.041569	-1.061294
11	1	0	-0.234385	1.776635	-1.671923
12	6	0	1.354617	-2.250158	1.231323
13	1	0	1.447082	-3.232979	0.774579
14	6	0	1.144536	0.305447	2.380674
15	1	0	1.102295	1.294190	2.827355
16	6	0	1.913173	-0.689944	2.999466
17	1	0	2.439499	-0.462147	3.922614
18	6	0	2.017196	-1.961585	2.431078
19	1	0	2.620883	-2.725848	2.913297
20	6	0	-2.755378	-1.786429	-0.687375
21	1	0	-2.650530	-2.785105	-1.106305
22	6	0	-4.026304	-1.263092	-0.412738

```
     23          1           0       -4.912144   -1.859818   -0.614143
     24          6           0       -4.154231    0.024059    0.113613
     25          1           0       -5.140226    0.432329    0.319179
     26          6           0       -3.016924    0.801955    0.375359
     27          1           0       -3.137636    1.808720    0.764404
     28          6           0        1.814651   -0.570804   -2.048876
     29          6           0        1.764436    1.466123   -0.983791
     30          8           0        2.563669    0.510808   -1.607526
     31          8           0        2.245820    2.436358   -0.472825
     32          8           0        2.325554   -1.506432   -2.599039
     33          6           0       -0.613811    2.356864    0.951381
     34          1           0       -0.567129    2.431566    2.054914
     35          8           0       -0.850564    3.339298    0.282737
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3737283      0.2669735
0.2546219
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1926.8657465707 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1032.18943624     A.U. after   15 cycles
            Convg  =    0.2256D-08             -V/T =  2.0094
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000851673    0.000077569    0.000012511
      2        6           0.000199560    0.000094634   -0.000129834
```

3	1	0.000078754	0.000130215	-0.000061618
4	6	-0.000267451	-0.000562156	-0.000084450
5	6	-0.000049109	0.000101134	-0.000644307
6	1	-0.000177488	0.000064334	0.000190953
7	6	0.000377333	0.000000916	0.000298240
8	6	0.000227791	-0.000105206	0.000469006
9	6	-0.001748111	-0.000204906	-0.000074256
10	6	-0.000405913	0.000635692	-0.000354662
11	1	-0.000186585	-0.000115212	0.000216735
12	6	0.000052756	0.000474681	0.000234026
13	1	-0.000054665	0.000171672	0.000060492
14	6	0.000218686	-0.000479305	-0.000203899
15	1	0.000052447	-0.000160607	-0.000051580
16	6	-0.000282784	-0.000206796	-0.000588720
17	1	-0.000104025	-0.000032563	-0.000111088
18	6	-0.000340614	0.000493730	-0.000290068
19	1	-0.000101225	0.000085879	-0.000061062
20	6	-0.000143473	0.000456951	0.000199281
21	1	-0.000002952	0.000172831	0.000060382
22	6	0.000582561	0.000354319	0.000141454
23	1	0.000121766	0.000074973	0.000023065
24	6	0.000636862	-0.000220037	-0.000190633
25	1	0.000137460	-0.000032291	-0.000005471
26	6	0.000098965	-0.000522007	-0.000273643
27	1	0.000136357	0.000006383	-0.000008114
28	6	0.001099683	-0.001207065	0.001761372
29	6	0.000573583	-0.000564723	0.002755527
30	8	-0.000501768	0.000328545	-0.001223224
31	8	-0.000671237	-0.000338711	-0.001117827
32	8	-0.000729732	0.000939509	-0.000247500
33	6	0.006201698	0.001989151	-0.001307052
34	1	-0.002160823	-0.000716540	0.000273229
35	8	-0.002016633	-0.001184992	0.000332736

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.006201698 RMS     0.000892140


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.001546692 RMS     0.000351492
 Search for a local minimum.
 Step number   4 out of a maximum of  210
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
 DE= -2.78D-05 DEPred=-2.08D-04 R= 1.34D-01
 Trust test= 1.34D-01 RLast= 1.26D-01 DXMaxT set to 1.50D-01
     Eigenvalues ---    0.00430   0.00471   0.00767   0.00990
0.01128
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.01162   0.01427   0.01476   0.01569
0.01797
     Eigenvalues ---    0.02105   0.02117   0.02121   0.02130
0.02132
     Eigenvalues ---    0.02134   0.02135   0.02142   0.02145
0.02156
     Eigenvalues ---    0.02159   0.02165   0.02574   0.03379
0.03658
     Eigenvalues ---    0.04152   0.04502   0.04774   0.05131
0.05233
     Eigenvalues ---    0.05345   0.05684   0.06280   0.06642
0.08044
     Eigenvalues ---    0.08523   0.09335   0.09915   0.12453
0.15056
     Eigenvalues ---    0.15999   0.15999   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16006   0.16025   0.16396
0.20192
     Eigenvalues ---    0.21275   0.21996   0.22000   0.22158
0.22607
     Eigenvalues ---    0.22614   0.22655   0.23816   0.24576
0.24654
     Eigenvalues ---    0.24732   0.25012   0.26796   0.27015
0.27604
     Eigenvalues ---    0.28788   0.28824   0.29669   0.29947
0.31036
     Eigenvalues ---    0.32407   0.34305   0.34404   0.34528
0.35121
     Eigenvalues ---    0.35157   0.35233   0.35244   0.35248
0.35266
     Eigenvalues ---    0.35343   0.35366   0.36721   0.39930
0.41966
     Eigenvalues ---    0.42044   0.42439   0.43706   0.44214
0.45301
     Eigenvalues ---    0.46050   0.46175   0.46324   0.46418
0.46801
     Eigenvalues ---    0.47062   0.96141   1.03620
1.067321000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     4    3    2    1
 RFO step:  Lambda=-9.55632438D-05.
 DIIS coeffs:      0.15485      0.25220      0.32238      0.27057
 Iteration  1 RMS(Cart)=  0.00542676 RMS(Int)=  0.00007386
 Iteration  2 RMS(Cart)=  0.00007761 RMS(Int)=  0.00001773
 Iteration  3 RMS(Cart)=  0.00000001 RMS(Int)=  0.00001773
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86354   0.00002  -0.00015   0.00040   0.00025
2.86379
    R2        2.65817  -0.00059  -0.00052  -0.00019  -0.00071
2.65746
```

This journal is © The Royal Society of Chemistry 2014

R3	2.63273	-0.00077	-0.00117	-0.00001	-0.00118
2.63155					
R4	2.06515	-0.00009	-0.00020	0.00002	-0.00019
2.06496					
R5	2.97241	-0.00051	-0.00040	-0.00056	-0.00097
2.97144					
R6	2.86862	-0.00014	0.00035	-0.00058	-0.00023
2.86839					
R7	2.92145	-0.00032	-0.00138	0.00033	-0.00106
2.92039					
R8	2.63753	-0.00098	-0.00142	0.00001	-0.00141
2.63612					
R9	2.06775	-0.00007	-0.00033	0.00007	-0.00026
2.06749					
R10	2.91402	-0.00033	-0.00195	0.00081	-0.00115
2.91288					
R11	2.87192	-0.00017	0.00100	-0.00078	0.00023
2.87214					
R12	2.66255	-0.00040	-0.00042	-0.00022	-0.00064
2.66191					
R13	2.63419	-0.00075	-0.00120	0.00004	-0.00117
2.63303					
R14	2.89884	-0.00009	-0.00149	0.00066	-0.00083
2.89801					
R15	2.63891	-0.00064	-0.00111	0.00002	-0.00109
2.63782					
R16	2.98099	-0.00124	-0.00142	-0.00159	-0.00302
2.97797					
R17	2.88083	-0.00049	0.00004	-0.00111	-0.00107
2.87976					
R18	2.06812	-0.00011	-0.00069	0.00033	-0.00036
2.06776					
R19	2.88683	-0.00040	-0.00034	-0.00072	-0.00107
2.88576					
R20	2.05546	-0.00019	-0.00043	0.00003	-0.00039
2.05507					
R21	2.64676	-0.00079	-0.00126	0.00001	-0.00125
2.64551					
R22	2.05183	-0.00017	-0.00022	-0.00004	-0.00026
2.05157					
R23	2.64866	-0.00074	-0.00132	0.00010	-0.00121
2.64744					
R24	2.05374	-0.00015	-0.00027	-0.00003	-0.00030
2.05344					
R25	2.63951	-0.00079	-0.00143	0.00014	-0.00128
2.63822					
R26	2.05370	-0.00014	-0.00026	-0.00003	-0.00029
2.05341					
R27	2.05611	-0.00018	-0.00038	0.00000	-0.00038
2.05573					
R28	2.64869	-0.00077	-0.00145	0.00010	-0.00135
2.64734					

This journal is © The Royal Society of Chemistry 2014

R29	2.05395	-0.00014	-0.00026	-0.00003	-0.00028
2.05367					
R30	2.63897	-0.00067	-0.00128	0.00012	-0.00116
2.63782					
R31	2.05375	-0.00014	-0.00024	-0.00004	-0.00028
2.05347					
R32	2.65040	-0.00080	-0.00152	0.00013	-0.00139
2.64901					
R33	2.05234	-0.00001	-0.00024	-0.00002	-0.00026
2.05208					
R34	2.62237	-0.00028	0.00011	-0.00023	-0.00011
2.62226					
R35	2.26696	-0.00093	-0.00161	0.00061	-0.00100
2.26596					
R36	2.63239	0.00004	-0.00134	0.00071	-0.00063
2.63176					
R37	2.26308	-0.00101	-0.00086	0.00019	-0.00067
2.26241					
R38	2.09201	0.00010	0.00139	-0.00061	0.00078
2.09279					
R39	2.28986	-0.00072	-0.00138	0.00062	-0.00077
2.28909					
A1	1.98183	-0.00024	-0.00054	0.00034	-0.00020
1.98163					
A2	2.19817	0.00023	0.00093	-0.00050	0.00043
2.19861					
A3	2.10286	0.00001	-0.00045	0.00019	-0.00026
2.10259					
A4	1.97248	0.00005	0.00090	-0.00006	0.00083
1.97331					
A5	1.82725	-0.00004	0.00074	-0.00006	0.00068
1.82793					
A6	1.87765	0.00006	0.00057	0.00006	0.00062
1.87828					
A7	1.92823	0.00006	-0.00097	0.00016	-0.00081
1.92742					
A8	1.96594	0.00003	0.00009	0.00005	0.00014
1.96608					
A9	1.88505	-0.00018	-0.00136	-0.00016	-0.00151
1.88354					
A10	1.97587	0.00029	0.00024	-0.00033	-0.00008
1.97579					
A11	2.09353	0.00011	0.00037	0.00000	0.00038
2.09390					
A12	2.21377	-0.00040	-0.00065	0.00033	-0.00031
2.21346					
A13	1.89627	0.00004	0.00122	-0.00088	0.00033
1.89660					
A14	1.91491	0.00001	-0.00022	-0.00008	-0.00030
1.91461					
A15	1.96657	-0.00017	-0.00297	0.00150	-0.00147
1.96511					

This journal is © The Royal Society of Chemistry 2014

A16	1.97411	-0.00011	0.00015	-0.00005	0.00010
1.97421					
A17	1.88626	0.00020	0.00158	-0.00002	0.00156
1.88782					
A18	1.82633	0.00002	0.00012	-0.00038	-0.00026
1.82607					
A19	1.98917	0.00008	-0.00023	0.00005	-0.00017
1.98900					
A20	2.19031	-0.00008	0.00050	-0.00033	0.00017
2.19048					
A21	2.10367	0.00001	-0.00030	0.00029	-0.00002
2.10365					
A22	1.96968	-0.00011	-0.00018	0.00007	-0.00010
1.96958					
A23	2.08996	-0.00008	0.00020	-0.00021	-0.00001
2.08996					
A24	2.22249	0.00018	-0.00017	0.00017	0.00001
2.22250					
A25	1.86803	0.00000	0.00070	0.00049	0.00119
1.86922					
A26	1.84149	-0.00004	-0.00008	-0.00021	-0.00030
1.84119					
A27	1.91861	0.00021	0.00098	0.00053	0.00152
1.92013					
A28	1.85042	0.00003	0.00001	-0.00029	-0.00028
1.85014					
A29	2.01989	0.00012	0.00156	-0.00048	0.00109
2.02098					
A30	1.95477	-0.00032	-0.00321	-0.00003	-0.00324
1.95152					
A31	1.92429	0.00012	0.00055	0.00013	0.00069
1.92498					
A32	1.97805	-0.00007	0.00268	-0.00104	0.00164
1.97969					
A33	1.81503	0.00007	-0.00009	0.00046	0.00038
1.81541					
A34	1.89428	0.00001	-0.00171	0.00083	-0.00088
1.89340					
A35	1.96739	-0.00038	-0.00444	0.00052	-0.00392
1.96348					
A36	1.88513	0.00023	0.00301	-0.00096	0.00207
1.88720					
A37	2.09577	-0.00003	-0.00022	0.00014	-0.00009
2.09568					
A38	2.08647	-0.00001	-0.00008	-0.00005	-0.00013
2.08634					
A39	2.10093	0.00004	0.00031	-0.00008	0.00022
2.10116					
A40	2.11709	0.00006	-0.00068	0.00044	-0.00024
2.11685					
A41	2.08721	-0.00004	-0.00022	0.00004	-0.00018
2.08702					

This journal is © The Royal Society of Chemistry 2014

A42	2.07878	-0.00002	0.00091	-0.00047	0.00044
2.07922					
A43	2.08488	-0.00006	0.00001	-0.00010	-0.00010
2.08479					
A44	2.10336	0.00008	0.00007	0.00008	0.00015
2.10352					
A45	2.09488	-0.00003	-0.00007	0.00002	-0.00005
2.09482					
A46	2.09546	0.00004	0.00033	-0.00017	0.00016
2.09562					
A47	2.09206	-0.00003	-0.00018	0.00007	-0.00011
2.09195					
A48	2.09561	-0.00001	-0.00014	0.00010	-0.00004
2.09557					
A49	2.09617	0.00005	-0.00020	0.00010	-0.00010
2.09607					
A50	2.08622	-0.00013	-0.00007	-0.00008	-0.00015
2.08607					
A51	2.10079	0.00008	0.00027	-0.00002	0.00025
2.10104					
A52	2.09176	-0.00004	-0.00018	0.00001	-0.00018
2.09158					
A53	2.09562	0.00006	0.00035	-0.00012	0.00023
2.09585					
A54	2.09580	-0.00002	-0.00017	0.00011	-0.00006
2.09574					
A55	2.09515	0.00000	-0.00013	0.00011	-0.00002
2.09513					
A56	2.10281	0.00005	-0.00001	0.00012	0.00011
2.10292					
A57	2.08521	-0.00005	0.00014	-0.00023	-0.00009
2.08512					
A58	2.08517	-0.00009	-0.00020	-0.00012	-0.00032
2.08485					
A59	2.11408	-0.00009	-0.00138	0.00070	-0.00068
2.11339					
A60	2.08389	0.00019	0.00158	-0.00058	0.00100
2.08489					
A61	1.91711	-0.00003	-0.00035	0.00028	0.00000
1.91711					
A62	2.24370	-0.00025	-0.00089	0.00007	-0.00076
2.24294					
A63	2.12221	0.00029	0.00122	-0.00035	0.00093
2.12313					
A64	1.91460	-0.00007	0.00029	-0.00047	-0.00011
1.91449					
A65	2.25544	-0.00017	-0.00192	0.00057	-0.00127
2.25417					
A66	2.11301	0.00025	0.00151	-0.00007	0.00152
2.11453					
A67	1.94685	-0.00001	-0.00055	0.00018	-0.00036
1.94649					

This journal is © The Royal Society of Chemistry 2014

A68	2.03166	-0.00020	-0.00335	0.00080	-0.00243	2.02923
A69	2.15284	-0.00027	-0.00105	-0.00052	-0.00146	2.15138
A70	2.09854	0.00043	0.00174	-0.00030	0.00155	2.10009
D1	-3.14056	0.00007	0.00027	0.00042	0.00069	-3.13988
D2	-1.04111	0.00014	0.00006	0.00054	0.00059	-1.04052
D3	0.96127	-0.00006	-0.00089	0.00036	-0.00053	0.96074
D4	-0.02660	0.00003	-0.00193	0.00125	-0.00068	-0.02728
D5	2.07286	0.00010	-0.00214	0.00137	-0.00077	2.07209
D6	-2.20794	-0.00009	-0.00309	0.00119	-0.00190	-2.20984
D7	-0.02767	0.00002	0.00067	-0.00052	0.00016	-0.02751
D8	3.10839	-0.00007	-0.00294	0.00029	-0.00265	3.10574
D9	3.13987	0.00005	0.00271	-0.00128	0.00143	3.14130
D10	-0.00725	-0.00004	-0.00090	-0.00048	-0.00137	-0.00863
D11	0.02439	0.00004	0.00232	-0.00094	0.00138	0.02577
D12	-3.12039	0.00005	0.00274	-0.00079	0.00195	-3.11844
D13	3.13660	0.00000	-0.00002	-0.00005	-0.00007	3.13653
D14	-0.00819	0.00001	0.00041	0.00009	0.00050	-0.00769
D15	-1.09291	0.00003	-0.00253	0.00005	-0.00248	-1.09539
D16	1.07342	-0.00007	-0.00168	-0.00066	-0.00233	1.07108
D17	3.10062	-0.00015	-0.00346	-0.00027	-0.00373	3.09689
D18	1.03578	0.00009	-0.00154	0.00002	-0.00152	1.03426
D19	-3.08108	-0.00001	-0.00069	-0.00068	-0.00137	-3.08245
D20	-1.05388	-0.00008	-0.00247	-0.00030	-0.00276	-1.05664
D21	-3.09010	0.00005	-0.00294	0.00008	-0.00286	-3.09296
D22	-0.92378	-0.00005	-0.00208	-0.00062	-0.00271	-0.92649
D23	1.10343	-0.00012	-0.00387	-0.00024	-0.00411	1.09933

This journal is © The Royal Society of Chemistry 2014

D24	-0.93658	0.00002	0.00033	-0.00023	0.00010	-0.93647
D25	2.21499	0.00004	0.00282	-0.00103	0.00178	2.21678
D26	-3.12184	-0.00011	-0.00130	-0.00023	-0.00152	-3.12337
D27	0.02973	-0.00009	0.00119	-0.00103	0.00016	0.02989
D28	1.02702	-0.00008	0.00082	-0.00035	0.00047	1.02749
D29	-2.10459	-0.00005	0.00330	-0.00115	0.00215	-2.10245
D30	-0.92258	0.00000	-0.00064	0.00092	0.00028	-0.92230
D31	1.04295	0.00001	-0.00038	0.00071	0.00034	1.04329
D32	-3.12944	-0.00029	-0.00373	0.00084	-0.00288	-3.13232
D33	2.22500	0.00009	0.00325	0.00006	0.00331	2.22831
D34	-2.09265	0.00010	0.00352	-0.00016	0.00337	-2.08928
D35	0.01814	-0.00019	0.00017	-0.00002	0.00015	0.01829
D36	0.01741	0.00004	0.00063	0.00055	0.00117	0.01859
D37	-3.11319	0.00004	0.00087	0.00058	0.00145	-3.11174
D38	-3.13053	-0.00006	-0.00351	0.00147	-0.00204	-3.13258
D39	0.02205	-0.00006	-0.00326	0.00150	-0.00177	0.02028
D40	-0.08560	0.00009	0.00229	0.00059	0.00289	-0.08271
D41	-2.21284	0.00003	0.00220	0.00016	0.00236	-2.21048
D42	2.02771	-0.00025	-0.00273	0.00155	-0.00117	2.02654
D43	2.03465	0.00008	0.00380	-0.00063	0.00316	2.03781
D44	-0.09259	0.00002	0.00371	-0.00107	0.00264	-0.08996
D45	-2.13523	-0.00026	-0.00122	0.00032	-0.00090	-2.13613
D46	-2.19962	0.00028	0.00585	-0.00092	0.00493	-2.19469
D47	1.95633	0.00022	0.00576	-0.00136	0.00440	1.96073
D48	-0.08631	-0.00006	0.00083	0.00003	0.00087	-0.08544
D49	-2.02008	-0.00018	-0.00755	0.00083	-0.00671	-2.02679

This journal is © The Royal Society of Chemistry 2014

D50	1.10168	0.00046	0.00841	0.00074	0.00916	1.11083
D51	2.16767	-0.00026	-0.00828	0.00102	-0.00726	2.16042
D52	-0.99375	0.00038	0.00768	0.00093	0.00861	-0.98514
D53	0.05942	-0.00025	-0.00931	0.00130	-0.00801	0.05141
D54	-3.10200	0.00039	0.00665	0.00120	0.00785	-3.09415
D55	-0.02376	-0.00003	0.00000	0.00070	0.00071	-0.02305
D56	-3.11971	0.00004	0.00302	-0.00011	0.00291	-3.11680
D57	3.10840	-0.00006	-0.00234	0.00146	-0.00088	3.10752
D58	0.01245	0.00002	0.00068	0.00064	0.00132	0.01378
D59	0.00128	-0.00004	-0.00327	0.00091	-0.00236	-0.00108
D60	3.13699	-0.00001	-0.00288	0.00105	-0.00183	3.13517
D61	-3.12973	-0.00001	-0.00064	0.00006	-0.00058	-3.13031
D62	0.00599	0.00002	-0.00025	0.00020	-0.00004	0.00594
D63	0.94741	-0.00008	0.00006	-0.00075	-0.00069	0.94672
D64	-1.01202	-0.00004	-0.00016	-0.00059	-0.00075	-1.01277
D65	3.09261	0.00027	0.00296	0.00000	0.00295	3.09556
D66	-2.24403	-0.00017	-0.00323	0.00013	-0.00310	-2.24713
D67	2.07973	-0.00013	-0.00344	0.00028	-0.00316	2.07657
D68	-0.09883	0.00018	-0.00033	0.00087	0.00055	-0.09829
D69	3.10324	-0.00004	-0.00061	-0.00022	-0.00083	3.10242
D70	-0.02270	-0.00004	-0.00072	-0.00105	-0.00177	-0.02446
D71	0.01456	0.00006	0.00288	-0.00115	0.00173	0.01629
D72	-3.11138	0.00005	0.00277	-0.00198	0.00079	-3.11059
D73	-0.93522	0.00002	-0.00155	-0.00080	-0.00235	-0.93757
D74	1.24086	0.00003	0.00102	-0.00146	-0.00043	1.24043
D75	-2.95492	0.00008	0.00091	-0.00178	-0.00087	-2.95578

This journal is © The Royal Society of Chemistry 2014

D76	1.04263	0.00001	-0.00079	-0.00046	-0.00126	1.04138
D77	-3.06447	0.00002	0.00178	-0.00112	0.00066	-3.06381
D78	-0.97706	0.00007	0.00167	-0.00144	0.00022	-0.97684
D79	-3.02227	-0.00003	-0.00093	-0.00130	-0.00223	-3.02450
D80	-0.84619	-0.00002	0.00164	-0.00196	-0.00031	-0.84650
D81	1.24122	0.00003	0.00153	-0.00228	-0.00075	1.24047
D82	1.65189	-0.00130	-0.02276	-0.00769	-0.03045	1.62144
D83	-1.47142	0.00154	0.03301	-0.00609	0.02692	-1.44450
D84	-0.46640	-0.00155	-0.02561	-0.00841	-0.03401	-0.50042
D85	2.69347	0.00130	0.03016	-0.00681	0.02336	2.71683
D86	-2.59009	-0.00142	-0.02420	-0.00763	-0.03183	-2.62193
D87	0.56978	0.00143	0.03157	-0.00603	0.02554	0.59532
D88	0.08948	0.00035	0.00791	-0.00141	0.00649	0.09598
D89	-3.03403	-0.00043	-0.00946	-0.00343	-0.01290	-3.04693
D90	2.17369	0.00034	0.00622	-0.00069	0.00552	2.17921
D91	-0.94982	-0.00043	-0.01115	-0.00271	-0.01388	-0.96369
D92	-2.01679	0.00027	0.00337	0.00002	0.00339	-2.01340
D93	1.14288	-0.00050	-0.01400	-0.00200	-0.01600	1.12688
D94	-0.01403	-0.00003	-0.00013	-0.00064	-0.00077	-0.01481
D95	3.13885	-0.00003	-0.00065	-0.00018	-0.00083	3.13802
D96	3.12167	0.00000	0.00026	-0.00049	-0.00024	3.12143
D97	-0.00863	0.00000	-0.00026	-0.00004	-0.00030	-0.00893
D98	-3.13897	0.00004	0.00080	0.00063	0.00143	-3.13754
D99	0.01477	0.00004	0.00035	0.00062	0.00097	0.01574
D100	0.01793	0.00003	0.00071	-0.00019	0.00052	0.01845
D101	-3.11151	0.00003	0.00025	-0.00020	0.00005	-3.11146

```
   D102        0.00370   0.00000   0.00009   0.00023   0.00032
0.00402
   D103        3.13397   0.00000   0.00060  -0.00023   0.00037
3.13435
   D104       -3.12567   0.00000  -0.00037   0.00022  -0.00016  -
3.12583
   D105        0.00460   0.00000   0.00014  -0.00024  -0.00010
0.00451
   D106       -3.13258   0.00000  -0.00004  -0.00020  -0.00024  -
3.13282
   D107        0.01333   0.00002   0.00035   0.00022   0.00056
0.01390
   D108        0.00581   0.00001   0.00039  -0.00006   0.00033
0.00613
   D109       -3.13146   0.00004   0.00077   0.00036   0.00113  -
3.13033
   D110        3.13331  -0.00002  -0.00031  -0.00027  -0.00058
3.13272
   D111       -0.00311  -0.00002  -0.00062  -0.00014  -0.00076  -
0.00387
   D112       -0.00395   0.00001   0.00008   0.00015   0.00022  -
0.00373
   D113       -3.14037   0.00000  -0.00023   0.00028   0.00005  -
3.14032
   D114       -0.01231  -0.00001   0.00013  -0.00024  -0.00011  -
0.01243
   D115        3.11848  -0.00001  -0.00014  -0.00026  -0.00040
3.11809
   D116        3.13442  -0.00001  -0.00018  -0.00011  -0.00029
3.13414
   D117       -0.01797  -0.00002  -0.00044  -0.00013  -0.00057  -
0.01854
   D118       -0.00343   0.00049   0.01509  -0.00233   0.01276
0.00933
   D119       -3.12681  -0.00009   0.00043  -0.00224  -0.00180  -
3.12862
   D120       -0.05615  -0.00053  -0.01451   0.00236  -0.01214  -
0.06829
   D121        3.06909   0.00017   0.00121   0.00419   0.00540
3.07449
         Item               Value     Threshold  Converged?
 Maximum Force            0.001547     0.000450     NO
 RMS     Force            0.000351     0.000300     NO
 Maximum Displacement     0.046436     0.001800     NO
 RMS     Displacement     0.005441     0.001200     NO
 Predicted change in Energy=-1.815361D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.619996	-1.033824	-0.393018
2	6	0	-0.184769	-1.436144	-0.666614
3	1	0	-0.093725	-2.444926	-1.076653
4	6	0	-1.748937	0.263956	0.133034
5	6	0	0.338036	-0.373768	-1.701279
6	1	0	-0.251321	-0.459290	-2.619064
7	6	0	0.596404	-1.256437	0.622358
8	6	0	0.479462	0.028422	1.187759
9	6	0	-0.391877	0.971138	0.348793
10	6	0	0.281348	1.033413	-1.074678
11	1	0	-0.264029	1.759714	-1.684880
12	6	0	1.385836	-2.229046	1.232458
13	1	0	1.479232	-3.215310	0.783893
14	6	0	1.172912	0.335079	2.359748
15	1	0	1.129535	1.327752	2.797172
16	6	0	1.955437	-0.648958	2.977838
17	1	0	2.491349	-0.409081	3.892182
18	6	0	2.060748	-1.924678	2.420607
19	1	0	2.675148	-2.680276	2.902606
20	6	0	-2.749140	-1.808356	-0.646688
21	1	0	-2.642570	-2.809752	-1.058094
22	6	0	-4.019641	-1.289488	-0.365332
23	1	0	-4.903871	-1.892574	-0.553637
24	6	0	-4.149928	0.001271	0.149863
25	1	0	-5.136185	0.406118	0.360107
26	6	0	-3.015309	0.787255	0.394609
27	1	0	-3.137141	1.797084	0.774888
28	6	0	1.801606	-0.576625	-2.057405
29	6	0	1.743577	1.469065	-1.010987
30	8	0	2.544266	0.518426	-1.639240
31	8	0	2.218525	2.453178	-0.521839
32	8	0	2.313335	-1.510282	-2.608990
33	6	0	-0.615068	2.361653	0.930975
34	1	0	-0.587120	2.440917	2.035237
35	8	0	-0.889137	3.328810	0.255088

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515451	0.000000			
3	H	2.188166	1.092731	0.000000		
4	C	1.406268	2.444668	3.397221	0.000000	
5	C	2.445631	1.572419	2.205963	2.850763	0.000000
6	H	2.675564	2.184201	2.519250	3.215584	1.094068
7	C	2.448056	1.517886	2.185274	2.837545	2.499029
8	C	2.834598	2.454559	3.401993	2.476627	2.920325
9	C	2.465448	2.620869	3.713527	1.545403	2.558191
10	C	2.890197	2.546074	3.498503	2.484489	1.541428
11	H	3.363244	3.355094	4.251816	2.783353	2.216866

This journal is © The Royal Society of Chemistry 2014

12	C	3.620187	2.588816	2.750945	4.153383	3.625845
13	H	3.968528	2.835190	2.555253	4.790615	3.943700
14	C	4.153547	3.760240	4.598005	3.674305	4.206117
15	H	4.828486	4.622157	5.544004	4.063852	4.874187
16	C	4.928947	4.299091	4.885025	4.759067	4.958413
17	H	5.971298	5.385081	5.959580	5.706505	5.993731
18	C	4.717837	3.848629	4.140439	4.953465	4.728953
19	H	5.658640	4.739866	4.853509	5.992626	5.654894
20	C	1.392556	2.591319	2.764293	2.429578	3.563826
21	H	2.154508	2.842681	2.574889	3.415413	3.902783
22	C	2.413384	3.849483	4.153773	2.796007	4.648940
23	H	3.398099	4.742468	4.869922	3.882750	5.576866
24	C	2.786879	4.295961	4.892955	2.415377	4.869210
25	H	3.873527	5.381877	5.968176	3.397825	5.901239
26	C	2.425609	3.752553	4.598615	1.394977	4.121364
27	H	3.417568	4.609576	5.539425	2.165541	4.787573
28	C	3.832307	2.572695	2.836319	4.255697	1.519873
29	C	4.237920	3.503905	4.324270	3.867651	2.418280
30	O	4.615586	3.494851	4.007113	4.651592	2.380611
31	O	5.187487	4.574234	5.444791	4.578461	3.594293
32	O	4.539674	3.165256	3.002591	5.212358	2.453041
33	C	3.780490	4.142549	5.235033	2.514498	3.914038
34	H	4.363150	4.742730	5.813670	3.115663	4.768639
35	O	4.470657	4.904127	5.978482	3.185511	4.363761

		6	7	8	9	10
6	H	0.000000				
7	C	3.443965	0.000000			
8	C	3.906892	1.408622	0.000000		
9	C	3.297583	2.452269	1.533560	0.000000	
10	C	2.212922	2.867508	2.483521	1.575874	0.000000
11	H	2.407662	3.893694	3.435434	2.184954	1.094210
12	C	4.543846	1.393339	2.433038	3.765940	4.145649
13	H	4.708564	2.154684	3.418252	4.606160	4.789661
14	C	5.239087	2.425656	1.395876	2.626228	3.616330
15	H	5.868211	3.419368	2.168194	2.904553	3.974579
16	C	6.019225	2.786448	2.416968	3.878978	4.696364
17	H	7.065486	3.873058	3.398971	4.772169	5.624464
18	C	5.735094	2.413410	2.799104	4.323601	4.912594
19	H	6.632182	3.398239	3.885716	5.409383	5.944792
20	C	3.456783	3.620464	4.142803	3.777996	4.176443
21	H	3.698563	3.965812	4.779767	4.619532	4.829025
22	C	4.468644	4.720646	4.938715	4.333714	4.939387
23	H	5.288338	5.660447	5.975195	5.419715	5.976568
24	C	4.803979	4.932824	4.744388	3.886279	4.711796
25	H	5.786734	5.974566	5.688861	4.777848	5.639305
26	C	4.275012	4.156082	3.663104	2.630268	3.617643
27	H	4.993805	4.825620	4.047028	2.898313	3.961080
28	C	2.131604	3.015921	3.556014	3.605097	2.422635
29	C	3.206880	3.378192	2.916835	2.580135	1.527077
30	O	3.119501	3.472626	3.534890	3.574655	2.388460
31	O	4.356714	4.207339	3.438970	3.125483	2.464553
32	O	2.771668	3.667956	4.488431	4.714244	3.599093

This journal is © The Royal Society of Chemistry 2014

33	C	4.548935	3.827987	2.589961	1.523904	2.567183
34	H	5.494222	4.131269	2.770550	2.245543	3.522339
35	O	4.797631	4.833861	3.692628	2.411362	2.899511
		11	12	13	14	15
11	H	0.000000				
12	C	5.209905	0.000000			
13	H	5.821053	1.087498	0.000000		
14	C	4.522544	2.809067	3.896462	0.000000	
15	H	4.713534	3.894205	4.981465	1.085643	0.000000
16	C	5.698129	2.422288	3.409741	1.400968	2.149916
17	H	6.587822	3.407135	4.308221	2.154160	2.463772
18	C	5.986180	1.399945	2.163961	2.428674	3.404007
19	H	7.028321	2.157622	2.491069	3.412297	4.297014
20	C	4.470429	4.561380	4.680300	5.386600	6.061309
21	H	5.189444	4.670321	4.532840	6.010783	6.797852
22	C	5.014326	5.714445	5.938611	6.085054	6.585240
23	H	6.012241	6.547041	6.654518	7.097713	7.615799
24	C	4.643126	6.065559	6.514279	5.773010	6.053142
25	H	5.454548	7.088148	7.553679	6.618785	6.785863
26	C	3.583224	5.400938	6.031000	4.648379	4.821221
27	H	3.782410	6.072595	6.814328	4.819315	4.744937
28	C	3.140717	3.704936	3.890958	4.553867	5.257875
29	C	2.137543	4.340167	5.023429	3.601866	3.859935
30	O	3.070733	4.139712	4.576752	4.231565	4.726334
31	O	2.827832	5.068940	5.863723	3.726017	3.669922
32	O	4.264933	4.016665	3.887737	5.421650	6.219519
33	C	2.707076	5.016874	5.959047	3.057003	2.755954
34	H	3.795747	5.132793	6.150494	2.763616	2.183251
35	O	2.572217	6.084449	6.979565	4.200485	3.813327
		16	17	18	19	20
16	C	0.000000				
17	H	1.086631	0.000000			
18	C	1.396087	2.155919	0.000000		
19	H	2.156362	2.484225	1.086618	0.000000	
20	C	6.050987	7.072626	5.705861	6.540691	0.000000
21	H	6.488409	7.524997	5.916580	6.631895	1.087845
22	C	6.876673	7.829083	6.718337	7.578516	1.400913
23	H	7.814602	8.755303	7.573181	8.367055	2.158383
24	C	6.759862	7.634128	6.887529	7.832622	2.423108
25	H	7.632615	8.445080	7.840543	8.775366	3.408154
26	C	5.783087	6.632309	6.101279	7.120051	2.809331
27	H	6.063866	6.801808	6.601360	7.639152	3.894948
28	C	5.038112	5.991778	4.683694	5.458034	4.921034
29	C	4.521243	5.303552	4.836727	5.779366	5.573034
30	O	4.798638	5.608895	4.762867	5.556725	5.866790
31	O	4.684038	5.267879	5.277169	6.187704	6.546293
32	O	5.664153	6.596179	5.052957	5.646015	5.437658
33	C	4.456560	5.108379	5.267982	6.335132	4.942900
34	H	4.111012	4.587778	5.120365	6.133624	5.470226
35	O	5.597108	6.215141	6.402377	7.471453	5.537444
		21	22	23	24	25
21	H	0.000000				

22	C	2.165051	0.000000			
23	H	2.491821	1.086753	0.000000		
24	C	3.410739	1.395873	2.156384	0.000000	
25	H	4.309435	2.155925	2.484529	1.086649	0.000000
26	C	3.897145	2.428797	3.412817	1.401796	2.155127
27	H	4.982706	3.406734	4.301149	2.154376	2.470426
28	C	5.073084	6.103950	6.996889	6.373912	7.412361
29	C	6.127706	6.421929	7.463132	6.183478	7.095130
30	O	6.190135	6.926491	7.903556	6.948423	7.937212
31	O	7.184445	7.276453	8.343566	6.857130	7.685053
32	O	5.353027	6.722302	7.513899	7.188173	8.245209
33	C	5.900050	5.157748	6.220639	4.321664	4.958881
34	H	6.431415	5.608998	6.641969	4.711700	5.257420
35	O	6.517739	5.613703	6.635885	4.660080	5.156604

		26	27	28	29	30
26	C	0.000000				
27	H	1.085914	0.000000			
28	C	5.574514	6.168274	0.000000		
29	C	5.008748	5.207529	2.298522	0.000000	
30	O	5.926018	6.304075	1.387639	1.392666	0.000000
31	O	5.568500	5.549335	3.422205	1.197214	2.257866
32	O	6.534121	7.217824	1.199095	3.428520	2.260398
33	C	2.920201	2.589199	4.837790	3.182945	4.470446
34	H	3.364871	2.916438	5.617943	3.956782	5.196473
35	O	3.316560	2.769458	5.276377	3.463060	4.824417

		31	32	33	34	35
31	O	0.000000				
32	O	4.480425	0.000000			
33	C	3.185639	6.008226	0.000000		
34	H	3.796108	6.752293	1.107456	0.000000	
35	O	3.320831	6.471135	1.211334	2.012088	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.621609	-1.023582	-0.416971
2	6	0	-0.185597	-1.428010	-0.683247
3	1	0	-0.094831	-2.431837	-1.105330
4	6	0	-1.750179	0.267889	0.124473
5	6	0	0.350242	-0.354600	-1.699695
6	1	0	-0.231423	-0.426115	-2.623566
7	6	0	0.585003	-1.267798	0.614630
8	6	0	0.468038	0.010205	1.195359
9	6	0	-0.392364	0.966938	0.360987
10	6	0	0.293462	1.044697	-1.055691

11	1	0	-0.243809	1.780844	-1.661268
12	6	0	1.365380	-2.251186	1.219073
13	1	0	1.458920	-3.232016	0.758775
14	6	0	1.152420	0.299188	2.377128
15	1	0	1.109019	1.286372	2.826801
16	6	0	1.925779	-0.695702	2.989354
17	1	0	2.454619	-0.469592	3.911292
18	6	0	2.031076	-1.964624	2.416810
19	1	0	2.638372	-2.728703	2.894423
20	6	0	-2.751443	-1.790387	-0.690278
21	1	0	-2.645112	-2.786873	-1.113500
22	6	0	-4.022360	-1.270168	-0.413330
23	1	0	-4.907208	-1.867334	-0.616969
24	6	0	-4.152209	0.014427	0.117158
25	1	0	-5.138709	0.420427	0.324008
26	6	0	-3.016777	0.792775	0.381735
27	1	0	-3.138067	1.798148	0.773809
28	6	0	1.816074	-0.558643	-2.045698
29	6	0	1.756731	1.473766	-0.973785
30	8	0	2.559232	0.528073	-1.607170
31	8	0	2.231148	2.449700	-0.468016
32	8	0	2.329025	-1.487199	-2.604709
33	6	0	-0.615316	2.350791	0.958924
34	1	0	-0.596682	2.415874	2.064308
35	8	0	-0.879803	3.327545	0.293094

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3744950      0.2671851
0.2546510
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1927.7183441850 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
```

This journal is © The Royal Society of Chemistry 2014

```
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1032.18960831     A.U. after   13 cycles
             Convg  =    0.8874D-08             -V/T =  2.0093
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000146525    0.000048422    0.000012033
      2        6           0.000051327    0.000043276   -0.000038414
      3        1          -0.000007754    0.000019190   -0.000012590
      4        6          -0.000108576   -0.000076573    0.000094159
      5        6           0.000064937   -0.000126053   -0.000048796
      6        1          -0.000012480    0.000027158    0.000015048
      7        6           0.000056504    0.000013622    0.000078446
      8        6           0.000077341   -0.000086032    0.000075222
      9        6           0.000057707    0.000108128   -0.000237336
     10        6          -0.000079918    0.000058177    0.000219839
     11        1           0.000013664    0.000000716    0.000024372
     12        6          -0.000002831    0.000070431    0.000041954
     13        1          -0.000009668    0.000030444    0.000004059
     14        6          -0.000010421   -0.000072422   -0.000036874
     15        1          -0.000000274    0.000008417   -0.000007630
     16        6          -0.000035896   -0.000037430   -0.000111363
     17        1          -0.000013983   -0.000003565   -0.000021590
     18        6          -0.000044236    0.000087492   -0.000052335
     19        1          -0.000019650    0.000012816   -0.000008244
     20        6          -0.000021264    0.000069412    0.000034343
     21        1           0.000000888    0.000036744    0.000008394
     22        6           0.000088837    0.000069938    0.000026832
     23        1           0.000019244    0.000013970    0.000013039
     24        6           0.000111125   -0.000054654   -0.000049208
     25        1           0.000023099    0.000000146    0.000005652
     26        6           0.000056316   -0.000087838   -0.000028586
     27        1           0.000022264    0.000008444    0.000002336
     28        6           0.000135325    0.000096491    0.000152629
     29        6          -0.000054356    0.000278205    0.000084887
     30        8          -0.000018830   -0.000206814   -0.000100819
     31        8          -0.000100931   -0.000256368   -0.000074057
     32        8          -0.000093690    0.000065382   -0.000001859
     33        6          -0.000007251   -0.000013254   -0.000127644
     34        1          -0.000005637   -0.000088540    0.000064631
     35        8           0.000015595   -0.000057475   -0.000000527
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000278205 RMS     0.000078912

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
```

This journal is © The Royal Society of Chemistry 2014

```
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000280467 RMS     0.000048708
 Search for a local minimum.
 Step number   5 out of a maximum of  210
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
 DE= -1.72D-04 DEPred=-1.82D-04 R= 9.48D-01
 SS=  1.41D+00  RLast= 8.28D-02 DXNew= 2.5227D-01 2.4829D-01
 Trust test= 9.48D-01 RLast= 8.28D-02 DXMaxT set to 2.48D-01
     Eigenvalues ---    0.00440   0.00464   0.00774   0.01086
0.01133
     Eigenvalues ---    0.01165   0.01428   0.01476   0.01571
0.01801
     Eigenvalues ---    0.02115   0.02120   0.02128   0.02131
0.02132
     Eigenvalues ---    0.02134   0.02142   0.02143   0.02152
0.02156
     Eigenvalues ---    0.02160   0.02165   0.02750   0.03400
0.03877
     Eigenvalues ---    0.04154   0.04710   0.04918   0.05239
0.05310
     Eigenvalues ---    0.05344   0.05812   0.06428   0.06657
0.08202
     Eigenvalues ---    0.08640   0.09345   0.09991   0.12421
0.15748
     Eigenvalues ---    0.15998   0.15999   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16006   0.16011   0.16407
0.20260
     Eigenvalues ---    0.21784   0.21995   0.22000   0.22218
0.22613
     Eigenvalues ---    0.22623   0.22808   0.24423   0.24536
0.24619
     Eigenvalues ---    0.24906   0.25019   0.26621   0.27074
0.27698
     Eigenvalues ---    0.28797   0.28878   0.29739   0.29932
0.30405
     Eigenvalues ---    0.32598   0.34377   0.34404   0.34528
0.35125
     Eigenvalues ---    0.35166   0.35233   0.35244   0.35248
0.35267
     Eigenvalues ---    0.35348   0.35393   0.36720   0.39930
0.42014
     Eigenvalues ---    0.42048   0.43336   0.44107   0.44758
0.45718
     Eigenvalues ---    0.46046   0.46152   0.46322   0.46383
0.46812
     Eigenvalues ---    0.47410   0.98442   1.04774
1.066291000.00000
```

```
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
      Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     5    4    3    2
1
 RFO step:  Lambda=-9.46821248D-07.
 DIIS coeffs:      0.85530      0.00745      0.02425      0.03766
0.07534
 Iteration  1 RMS(Cart)=  0.00075246 RMS(Int)=  0.00000188
 Iteration  2 RMS(Cart)=  0.00000048 RMS(Int)=  0.00000182
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                   (DIIS)     (GDIIS)  (Total)
    R1        2.86379   0.00003  -0.00003   0.00008   0.00005
2.86384
    R2        2.65746  -0.00011  -0.00005  -0.00023  -0.00028
2.65718
    R3        2.63155  -0.00013  -0.00015  -0.00010  -0.00025
2.63130
    R4        2.06496  -0.00001  -0.00003  -0.00001  -0.00004
2.06493
    R5        2.97144  -0.00010  -0.00002  -0.00020  -0.00022
2.97122
    R6        2.86839   0.00000   0.00006   0.00002   0.00008
2.86847
    R7        2.92039  -0.00008  -0.00019  -0.00014  -0.00032
2.92006
    R8        2.63612  -0.00020  -0.00018  -0.00021  -0.00039
2.63574
    R9        2.06749  -0.00001  -0.00005   0.00002  -0.00003
2.06746
   R10        2.91288  -0.00001  -0.00029   0.00035   0.00006
2.91293
   R11        2.87214  -0.00007   0.00016  -0.00034  -0.00018
2.87197
   R12        2.66191  -0.00012  -0.00005  -0.00016  -0.00021
2.66170
   R13        2.63303  -0.00012  -0.00015  -0.00009  -0.00024
2.63279
   R14        2.89801  -0.00005  -0.00023   0.00002  -0.00021
2.89780
   R15        2.63782  -0.00015  -0.00014  -0.00015  -0.00029
2.63754
   R16        2.97797  -0.00025  -0.00010  -0.00076  -0.00086
2.97711
   R17        2.87976  -0.00017   0.00005  -0.00052  -0.00047
2.87929
   R18        2.06776  -0.00002  -0.00010   0.00004  -0.00007
2.06769
   R19        2.88576  -0.00009  -0.00001  -0.00021  -0.00022
2.88554
   R20        2.05507  -0.00003  -0.00006  -0.00003  -0.00008
2.05499
   R21        2.64551  -0.00011  -0.00016  -0.00005  -0.00021
2.64530
```

This journal is © The Royal Society of Chemistry 2014

R22	2.05157	0.00001	-0.00002	0.00004	0.00002
2.05159					
R23	2.64744	-0.00013	-0.00017	-0.00009	-0.00026
2.64718					
R24	2.05344	-0.00002	-0.00003	-0.00003	-0.00006
2.05337					
R25	2.63822	-0.00012	-0.00019	-0.00005	-0.00024
2.63799					
R26	2.05341	-0.00002	-0.00003	-0.00003	-0.00006
2.05335					
R27	2.05573	-0.00003	-0.00005	-0.00004	-0.00009
2.05564					
R28	2.64734	-0.00012	-0.00019	-0.00006	-0.00025
2.64709					
R29	2.05367	-0.00002	-0.00003	-0.00003	-0.00006
2.05360					
R30	2.63782	-0.00012	-0.00017	-0.00007	-0.00024
2.63758					
R31	2.05347	-0.00002	-0.00003	-0.00002	-0.00005
2.05342					
R32	2.64901	-0.00013	-0.00020	-0.00006	-0.00026
2.64875					
R33	2.05208	0.00000	-0.00003	0.00004	0.00001
2.05209					
R34	2.62226	-0.00017	0.00003	-0.00038	-0.00035
2.62191					
R35	2.26596	-0.00009	-0.00024	0.00013	-0.00010
2.26586					
R36	2.63176	0.00011	-0.00021	0.00036	0.00015
2.63191					
R37	2.26241	-0.00028	-0.00012	-0.00012	-0.00024
2.26216					
R38	2.09279	0.00006	0.00021	-0.00003	0.00018
2.09297					
R39	2.28909	-0.00005	-0.00021	0.00014	-0.00007
2.28902					
A1	1.98163	-0.00003	-0.00008	-0.00003	-0.00010
1.98152					
A2	2.19861	0.00003	0.00014	-0.00001	0.00013
2.19874					
A3	2.10259	-0.00001	-0.00007	0.00005	-0.00002
2.10257					
A4	1.97331	0.00001	0.00012	-0.00011	0.00001
1.97332					
A5	1.82793	0.00001	0.00012	0.00000	0.00012
1.82805					
A6	1.87828	-0.00001	0.00007	-0.00006	0.00001
1.87829					
A7	1.92742	0.00000	-0.00013	0.00003	-0.00010
1.92732					
A8	1.96608	0.00001	0.00000	0.00014	0.00014
1.96622					

This journal is © The Royal Society of Chemistry 2014

A9	1.88354	-0.00002	-0.00018	-0.00001	-0.00019
1.88336					
A10	1.97579	0.00002	0.00003	0.00004	0.00006
1.97585					
A11	2.09390	0.00004	0.00005	0.00010	0.00015
2.09405					
A12	2.21346	-0.00006	-0.00008	-0.00014	-0.00022
2.21324					
A13	1.89660	0.00002	0.00019	0.00004	0.00023
1.89683					
A14	1.91461	-0.00002	-0.00003	-0.00005	-0.00008
1.91453					
A15	1.96511	-0.00001	-0.00044	0.00009	-0.00035
1.96476					
A16	1.97421	-0.00002	0.00006	-0.00022	-0.00016
1.97405					
A17	1.88782	0.00002	0.00018	0.00011	0.00029
1.88810					
A18	1.82607	0.00002	0.00002	0.00003	0.00005
1.82612					
A19	1.98900	-0.00001	-0.00004	-0.00001	-0.00005
1.98895					
A20	2.19048	0.00003	0.00009	0.00005	0.00013
2.19061					
A21	2.10365	-0.00002	-0.00005	-0.00004	-0.00009
2.10356					
A22	1.96958	0.00001	-0.00002	-0.00003	-0.00005
1.96953					
A23	2.08996	0.00004	0.00003	0.00015	0.00018
2.09014					
A24	2.22250	-0.00006	-0.00004	-0.00011	-0.00014
2.22235					
A25	1.86922	0.00000	0.00008	-0.00019	-0.00010
1.86912					
A26	1.84119	0.00004	0.00000	0.00046	0.00046
1.84165					
A27	1.92013	-0.00003	0.00010	-0.00043	-0.00033
1.91980					
A28	1.85014	0.00000	0.00001	-0.00004	-0.00002
1.85012					
A29	2.02098	-0.00001	0.00021	-0.00034	-0.00012
2.02086					
A30	1.95152	0.00001	-0.00042	0.00060	0.00018
1.95170					
A31	1.92498	0.00002	0.00006	-0.00006	0.00001
1.92499					
A32	1.97969	0.00001	0.00042	-0.00011	0.00031
1.98000					
A33	1.81541	-0.00003	0.00000	-0.00014	-0.00015
1.81526					
A34	1.89340	-0.00001	-0.00027	0.00025	-0.00002
1.89338					

This journal is © The Royal Society of Chemistry 2014

A35	1.96348	0.00000	-0.00059	0.00033	-0.00026
1.96322					
A36	1.88720	0.00002	0.00038	-0.00029	0.00010
1.88730					
A37	2.09568	0.00000	-0.00003	0.00000	-0.00003
2.09565					
A38	2.08634	-0.00001	-0.00001	-0.00004	-0.00005
2.08629					
A39	2.10116	0.00002	0.00004	0.00004	0.00008
2.10124					
A40	2.11685	0.00000	-0.00011	0.00010	-0.00001
2.11684					
A41	2.08702	-0.00003	-0.00003	-0.00011	-0.00014
2.08688					
A42	2.07922	0.00003	0.00014	0.00001	0.00015
2.07937					
A43	2.08479	-0.00001	0.00001	-0.00006	-0.00005
2.08474					
A44	2.10352	0.00001	0.00001	0.00002	0.00003
2.10355					
A45	2.09482	0.00000	-0.00001	0.00003	0.00002
2.09485					
A46	2.09562	0.00001	0.00005	0.00002	0.00007
2.09568					
A47	2.09195	0.00000	-0.00003	0.00001	-0.00002
2.09193					
A48	2.09557	-0.00001	-0.00002	-0.00002	-0.00005
2.09552					
A49	2.09607	0.00001	-0.00003	0.00003	0.00000
2.09607					
A50	2.08607	-0.00003	0.00000	-0.00008	-0.00009
2.08598					
A51	2.10104	0.00002	0.00004	0.00005	0.00009
2.10112					
A52	2.09158	0.00000	-0.00002	0.00001	-0.00002
2.09156					
A53	2.09585	0.00001	0.00005	-0.00001	0.00004
2.09589					
A54	2.09574	0.00000	-0.00003	0.00000	-0.00002
2.09572					
A55	2.09513	0.00000	-0.00002	0.00004	0.00002
2.09515					
A56	2.10292	0.00001	-0.00001	0.00005	0.00004
2.10297					
A57	2.08512	-0.00001	0.00003	-0.00009	-0.00006
2.08506					
A58	2.08485	-0.00003	-0.00002	-0.00010	-0.00012
2.08473					
A59	2.11339	-0.00001	-0.00021	0.00012	-0.00009
2.11330					
A60	2.08489	0.00004	0.00023	-0.00002	0.00021
2.08510					

This journal is © The Royal Society of Chemistry 2014

A61	1.91711	0.00003	-0.00006	0.00016	0.00010	1.91721
A62	2.24294	-0.00007	-0.00012	-0.00015	-0.00027	2.24267
A63	2.12313	0.00004	0.00016	0.00000	0.00017	2.12330
A64	1.91449	0.00000	0.00007	0.00004	0.00012	1.91461
A65	2.25417	0.00001	-0.00030	0.00023	-0.00006	2.25411
A66	2.11453	-0.00001	0.00020	-0.00026	-0.00005	2.11447
A67	1.94649	-0.00002	-0.00005	-0.00006	-0.00012	1.94637
A68	2.02923	-0.00010	-0.00034	-0.00025	-0.00058	2.02865
A69	2.15138	0.00001	-0.00009	0.00011	0.00003	2.15141
A70	2.10009	0.00009	0.00037	0.00013	0.00051	2.10060
D1	-3.13988	0.00000	0.00001	-0.00020	-0.00019	-3.14006
D2	-1.04052	0.00001	-0.00001	-0.00022	-0.00023	-1.04074
D3	0.96074	-0.00001	-0.00012	-0.00026	-0.00038	0.96036
D4	-0.02728	0.00001	-0.00031	0.00025	-0.00006	-0.02734
D5	2.07209	0.00002	-0.00033	0.00023	-0.00011	2.07198
D6	-2.20984	-0.00001	-0.00045	0.00019	-0.00026	-2.21010
D7	-0.02751	0.00002	0.00011	0.00052	0.00063	-0.02689
D8	3.10574	0.00000	-0.00039	0.00021	-0.00018	3.10557
D9	3.14130	0.00001	0.00041	0.00010	0.00051	-3.14137
D10	-0.00863	0.00000	-0.00009	-0.00020	-0.00029	-0.00892
D11	0.02577	0.00000	0.00034	-0.00041	-0.00007	0.02570
D12	-3.11844	0.00000	0.00039	-0.00035	0.00004	-3.11841
D13	3.13653	0.00000	0.00000	0.00006	0.00006	3.13659
D14	-0.00769	0.00000	0.00005	0.00012	0.00017	-0.00753
D15	-1.09539	0.00000	-0.00042	0.00034	-0.00008	-1.09547
D16	1.07108	-0.00002	-0.00024	0.00006	-0.00017	1.07091

This journal is © The Royal Society of Chemistry 2014

D17	3.09689	-0.00002	-0.00049	0.00012	-0.00037	3.09652
D18	1.03426	0.00001	-0.00028	0.00023	-0.00005	1.03421
D19	-3.08245	-0.00001	-0.00010	-0.00005	-0.00015	-3.08260
D20	-1.05664	-0.00001	-0.00035	0.00001	-0.00034	-1.05699
D21	-3.09296	0.00001	-0.00048	0.00042	-0.00006	-3.09302
D22	-0.92649	-0.00001	-0.00030	0.00014	-0.00016	-0.92664
D23	1.09933	-0.00001	-0.00055	0.00020	-0.00036	1.09897
D24	-0.93647	0.00001	0.00004	-0.00010	-0.00006	-0.93654
D25	2.21678	0.00001	0.00040	-0.00025	0.00015	2.21693
D26	-3.12337	0.00000	-0.00016	-0.00001	-0.00018	-3.12354
D27	0.02989	-0.00001	0.00020	-0.00016	0.00004	0.02992
D28	1.02749	0.00000	0.00013	-0.00014	-0.00001	1.02747
D29	-2.10245	0.00000	0.00049	-0.00029	0.00020	-2.10225
D30	-0.92230	-0.00002	-0.00012	-0.00049	-0.00061	-0.92291
D31	1.04329	0.00000	-0.00007	-0.00041	-0.00048	1.04282
D32	-3.13232	0.00001	-0.00051	0.00034	-0.00017	-3.13249
D33	2.22831	-0.00001	0.00042	-0.00016	0.00026	2.22857
D34	-2.08928	0.00001	0.00047	-0.00008	0.00039	-2.08889
D35	0.01829	0.00003	0.00003	0.00067	0.00070	0.01899
D36	0.01859	0.00000	0.00006	0.00009	0.00014	0.01873
D37	-3.11174	0.00001	0.00009	0.00028	0.00037	-3.11137
D38	-3.13258	-0.00002	-0.00052	-0.00026	-0.00078	-3.13336
D39	0.02028	-0.00001	-0.00048	-0.00007	-0.00055	0.01973
D40	-0.08271	0.00001	0.00033	-0.00021	0.00012	-0.08259
D41	-2.21048	0.00000	0.00034	-0.00042	-0.00008	-2.21056
D42	2.02654	-0.00001	-0.00034	0.00007	-0.00027	2.02627

This journal is © The Royal Society of Chemistry 2014

D43	2.03781	0.00000	0.00060	-0.00035	0.00025	2.03806
D44	-0.08996	0.00000	0.00060	-0.00056	0.00004	-0.08991
D45	-2.13613	-0.00001	-0.00007	-0.00007	-0.00014	-2.13627
D46	-2.19469	0.00002	0.00085	-0.00031	0.00054	-2.19415
D47	1.96073	0.00002	0.00086	-0.00052	0.00034	1.96107
D48	-0.08544	0.00001	0.00018	-0.00003	0.00016	-0.08528
D49	-2.02679	0.00001	-0.00033	0.00029	-0.00004	-2.02683
D50	1.11083	0.00004	-0.00044	0.00295	0.00251	1.11334
D51	2.16042	-0.00001	-0.00042	0.00012	-0.00030	2.16011
D52	-0.98514	0.00001	-0.00053	0.00277	0.00224	-0.98290
D53	0.05141	-0.00001	-0.00059	0.00030	-0.00029	0.05112
D54	-3.09415	0.00001	-0.00070	0.00295	0.00226	-3.09189
D55	-0.02305	0.00000	-0.00001	0.00012	0.00012	-0.02294
D56	-3.11680	0.00000	0.00040	-0.00010	0.00030	-3.11650
D57	3.10752	0.00000	-0.00035	0.00027	-0.00008	3.10744
D58	0.01378	0.00000	0.00006	0.00004	0.00010	0.01387
D59	-0.00108	0.00000	-0.00047	0.00016	-0.00031	-0.00139
D60	3.13517	0.00000	-0.00042	0.00003	-0.00039	3.13477
D61	-3.13031	0.00000	-0.00009	0.00000	-0.00008	-3.13039
D62	0.00594	0.00000	-0.00004	-0.00013	-0.00017	0.00577
D63	0.94672	0.00002	0.00003	0.00012	0.00015	0.94687
D64	-1.01277	-0.00002	-0.00001	-0.00030	-0.00031	-1.01308
D65	3.09556	-0.00002	0.00038	-0.00082	-0.00044	3.09512
D66	-2.24713	0.00002	-0.00041	0.00037	-0.00003	-2.24717
D67	2.07657	-0.00002	-0.00045	-0.00005	-0.00050	2.07607
D68	-0.09829	-0.00002	-0.00006	-0.00057	-0.00063	-0.09891

This journal is © The Royal Society of Chemistry 2014

D69	3.10242	0.00000	-0.00005	-0.00007	-0.00012	3.10230
D70	-0.02446	0.00000	-0.00004	0.00013	0.00008	-0.02438
D71	0.01629	0.00000	0.00042	-0.00033	0.00008	0.01638
D72	-3.11059	0.00001	0.00042	-0.00014	0.00029	-3.11030
D73	-0.93757	0.00000	-0.00022	0.00029	0.00007	-0.93750
D74	1.24043	0.00001	0.00017	0.00029	0.00046	1.24089
D75	-2.95578	0.00002	0.00010	0.00030	0.00041	-2.95537
D76	1.04138	0.00001	-0.00012	0.00027	0.00015	1.04152
D77	-3.06381	0.00003	0.00027	0.00026	0.00053	-3.06328
D78	-0.97684	0.00004	0.00020	0.00028	0.00048	-0.97636
D79	-3.02450	0.00000	-0.00011	0.00021	0.00010	-3.02440
D80	-0.84650	0.00001	0.00027	0.00021	0.00048	-0.84602
D81	1.24047	0.00003	0.00021	0.00022	0.00043	1.24090
D82	1.62144	-0.00004	0.00070	-0.00276	-0.00205	1.61938
D83	-1.44450	-0.00002	0.00105	-0.00263	-0.00158	-1.44607
D84	-0.50042	-0.00001	0.00035	-0.00192	-0.00157	-0.50199
D85	2.71683	0.00001	0.00070	-0.00179	-0.00109	2.71574
D86	-2.62193	-0.00001	0.00051	-0.00210	-0.00159	-2.62352
D87	0.59532	0.00001	0.00086	-0.00197	-0.00111	0.59421
D88	0.09598	-0.00001	0.00028	-0.00026	0.00002	0.09600
D89	-3.04693	0.00002	0.00068	0.00184	0.00253	-3.04440
D90	2.17921	-0.00001	0.00005	-0.00024	-0.00019	2.17902
D91	-0.96369	0.00002	0.00045	0.00186	0.00231	-0.96138
D92	-2.01340	-0.00001	-0.00040	0.00009	-0.00031	-2.01371
D93	1.12688	0.00002	0.00001	0.00219	0.00219	1.12907
D94	-0.01481	0.00000	0.00001	0.00005	0.00006	-0.01474

D95	3.13802	0.00000	-0.00008	-0.00006	-0.00013	3.13789
D96	3.12143	0.00000	0.00006	-0.00008	-0.00002	3.12141
D97	-0.00893	0.00000	-0.00003	-0.00019	-0.00022	-0.00915
D98	-3.13754	0.00000	0.00008	-0.00005	0.00003	-3.13751
D99	0.01574	-0.00001	0.00002	-0.00020	-0.00019	0.01555
D100	0.01845	0.00001	0.00009	0.00014	0.00023	0.01868
D101	-3.11146	0.00000	0.00002	-0.00001	0.00001	-3.11145
D102	0.00402	0.00000	0.00000	0.00011	0.00011	0.00413
D103	3.13435	0.00001	0.00009	0.00022	0.00031	3.13466
D104	-3.12583	0.00000	-0.00006	-0.00004	-0.00011	-3.12593
D105	0.00451	0.00000	0.00002	0.00007	0.00009	0.00460
D106	-3.13282	0.00000	0.00000	0.00005	0.00005	-3.13277
D107	0.01390	0.00000	0.00003	0.00008	0.00011	0.01401
D108	0.00613	0.00000	0.00005	0.00011	0.00016	0.00629
D109	-3.13033	0.00000	0.00008	0.00014	0.00022	-3.13011
D110	3.13272	0.00000	-0.00003	-0.00006	-0.00009	3.13263
D111	-0.00387	0.00000	-0.00007	-0.00019	-0.00026	-0.00413
D112	-0.00373	0.00000	0.00000	-0.00004	-0.00003	-0.00376
D113	-3.14032	0.00000	-0.00004	-0.00016	-0.00020	-3.14052
D114	-0.01243	0.00000	0.00002	0.00011	0.00013	-0.01230
D115	3.11809	0.00000	-0.00001	-0.00008	-0.00010	3.11799
D116	3.13414	0.00000	-0.00001	-0.00002	-0.00003	3.13410
D117	-0.01854	-0.00001	-0.00005	-0.00021	-0.00026	-0.01880
D118	0.00933	0.00000	0.00080	-0.00049	0.00032	0.00965
D119	-3.12862	-0.00002	0.00091	-0.00293	-0.00202	-3.13064
D120	-0.06829	0.00000	-0.00068	0.00046	-0.00022	-0.06851

```
   D121        3.07449  -0.00003  -0.00105  -0.00145  -0.00249
3.07200
         Item               Value     Threshold  Converged?
 Maximum Force            0.000280     0.000450     YES
 RMS     Force            0.000049     0.000300     YES
 Maximum Displacement     0.005649     0.001800     NO
 RMS     Displacement     0.000753     0.001200     YES
 Predicted change in Energy=-1.137286D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.620168   -1.033929   -0.393057
      2          6           0       -0.184917   -1.436255   -0.666680
      3          1           0       -0.093877   -2.444972   -1.076827
      4          6           0       -1.748915    0.263585    0.133304
      5          6           0        0.338034   -0.373966   -1.701187
      6          1           0       -0.251070   -0.459260   -2.619138
      7          6           0        0.596332   -1.256448    0.622284
      8          6           0        0.479430    0.028388    1.187467
      9          6           0       -0.391992    0.970833    0.348484
     10          6           0        0.281161    1.033206   -1.074511
     11          1           0       -0.263973    1.759756   -1.684571
     12          6           0        1.385906   -2.228744    1.232406
     13          1           0        1.479248   -3.215073    0.784082
     14          6           0        1.173017    0.335510    2.359073
     15          1           0        1.129620    1.328351    2.796137
     16          6           0        1.955839   -0.648181    2.977026
     17          1           0        2.491912   -0.408022    3.891162
     18          6           0        2.061074   -1.923931    2.420162
     19          1           0        2.675534   -2.679345    2.902299
     20          6           0       -2.749326   -1.808175   -0.646814
     21          1           0       -2.642923   -2.809450   -1.058433
     22          6           0       -4.019577   -1.289092   -0.365378
     23          1           0       -4.903914   -1.891956   -0.553696
     24          6           0       -4.149594    0.001555    0.149824
     25          1           0       -5.135736    0.406611    0.360056
     26          6           0       -3.014951    0.787178    0.394822
     27          1           0       -3.136398    1.797074    0.775056
     28          6           0        1.801681   -0.577049   -2.056471
     29          6           0        1.743342    1.468528   -1.010237
     30          8           0        2.544257    0.517808   -1.638255
     31          8           0        2.218430    2.451302   -0.518850
     32          8           0        2.312925   -1.509932   -2.609694
     33          6           0       -0.615552    2.360973    0.930774
     34          1           0       -0.589175    2.439168    2.035247
     35          8           0       -0.888691    3.328392    0.254951
```

This journal is © The Royal Society of Chemistry 2014

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515480	0.000000			
3	H	2.188183	1.092712	0.000000		
4	C	1.406121	2.444487	3.397035	0.000000	
5	C	2.445672	1.572304	2.205774	2.850821	0.000000
6	H	2.675838	2.184259	2.519223	3.215894	1.094053
7	C	2.448122	1.517929	2.185396	2.837214	2.498802
8	C	2.834587	2.454464	3.401943	2.476307	2.919966
9	C	2.465232	2.620593	3.713234	1.545232	2.557846
10	C	2.890066	2.545936	3.498340	2.484419	1.541457
11	H	3.363324	3.355121	4.251826	2.783567	2.217083
12	C	3.620248	2.588832	2.751194	4.152930	3.625494
13	H	3.968554	2.835198	2.555535	4.790157	3.943453
14	C	4.153488	3.760095	4.597989	3.673813	4.205504
15	H	4.828318	4.621921	5.543894	4.063295	4.873440
16	C	4.928903	4.298894	4.885030	4.758495	4.957637
17	H	5.971222	5.384849	5.959562	5.705889	5.992889
18	C	4.717822	3.848493	4.140559	4.952874	4.728296
19	H	5.658606	4.739732	4.853660	5.991988	5.654270
20	C	1.392425	2.591315	2.764386	2.429320	3.563769
21	H	2.154351	2.842698	2.575038	3.415118	3.902668
22	C	2.413097	3.849293	4.153713	2.795603	4.648722
23	H	3.397794	4.742295	4.869902	3.882312	5.576652
24	C	2.786565	4.295654	4.892750	2.414994	4.868887
25	H	3.873185	5.381538	5.967956	3.397416	5.900863
26	C	2.425408	3.752271	4.598393	1.394772	4.121167
27	H	3.417312	4.609150	5.539076	2.165305	4.787157
28	C	3.832067	2.572222	2.835839	4.255409	1.519780
29	C	4.237499	3.503424	4.323805	3.867225	2.418075
30	O	4.615283	3.494383	4.006622	4.651277	2.380471
31	O	5.186280	4.572858	5.443492	4.577252	3.593877
32	O	4.539744	3.165430	3.002779	5.212287	2.452753
33	C	3.779834	4.142010	5.234474	2.513863	3.913622
34	H	4.361423	4.741596	5.812499	3.113767	4.768058
35	O	4.470438	4.903729	5.978051	3.185565	4.363346

		6	7	8	9	10
6	H	0.000000				
7	C	3.443895	0.000000			
8	C	3.906619	1.408510	0.000000		
9	C	3.297242	2.452046	1.533450	0.000000	
10	C	2.212826	2.867221	2.483045	1.575418	0.000000
11	H	2.407823	3.893480	3.434950	2.184514	1.094175
12	C	4.543694	1.393211	2.432769	3.765572	4.145195
13	H	4.708546	2.154514	3.417952	4.605767	4.789327
14	C	5.238536	2.425557	1.395724	2.625900	3.615478
15	H	5.867458	3.419242	2.168056	2.904157	3.973526
16	C	6.018570	2.786226	2.416619	3.878498	4.695376
17	H	7.064742	3.872804	3.398603	4.771657	5.623385
18	C	5.734616	2.413166	2.798693	4.323082	4.911770

This journal is © The Royal Society of Chemistry 2014

19	H	6.631746	3.397968	3.885272	5.408834	5.943995
20	C	3.457009	3.620558	4.142755	3.777635	4.176149
21	H	3.698669	3.966031	4.779800	4.619161	4.828720
22	C	4.468746	4.720504	4.938436	4.333155	4.938855
23	H	5.288442	5.660345	5.974928	5.419126	5.976021
24	C	4.803955	4.932505	4.743974	3.885684	4.711145
25	H	5.786648	5.974206	5.688388	4.777194	5.638562
26	C	4.275114	4.155660	3.662615	2.629789	3.617157
27	H	4.993667	4.824998	4.046300	2.897654	3.960316
28	C	2.131726	3.014992	3.555001	3.604435	2.422632
29	C	3.206651	3.377314	2.915712	2.579433	1.526961
30	O	3.119399	3.471661	3.533801	3.574063	2.388524
31	O	4.356721	4.204854	3.436008	3.123838	2.464298
32	O	2.770934	3.668327	4.488492	4.713978	3.598944
33	C	4.548454	3.827475	2.589562	1.523657	2.566754
34	H	5.493496	4.130311	2.769929	2.245007	3.522046
35	O	4.797213	4.833320	3.692068	2.411129	2.898948

		11	12	13	14	15
11	H	0.000000				
12	C	5.209509	0.000000			
13	H	5.820823	1.087453	0.000000		
14	C	4.521556	2.808932	3.896282	0.000000	
15	H	4.712213	3.894080	4.981296	1.085652	0.000000
16	C	5.697035	2.422127	3.409557	1.400830	2.149892
17	H	6.586574	3.406943	4.308013	2.153979	2.463719
18	C	5.985334	1.399831	2.163869	2.428467	3.403865
19	H	7.027496	2.157481	2.490974	3.412038	4.296830
20	C	4.470352	4.561633	4.680562	5.386605	6.061182
21	H	5.189325	4.670828	4.533397	6.010950	6.797881
22	C	5.014011	5.714465	5.938664	6.084817	6.584863
23	H	6.011899	6.547169	6.654701	7.097529	7.615464
24	C	4.642663	6.065310	6.514050	5.772564	6.052558
25	H	5.453950	7.087871	7.553437	6.618269	6.785188
26	C	3.582968	5.400452	6.030536	4.647726	4.820441
27	H	3.781796	6.071871	6.813655	4.818333	4.743772
28	C	3.141002	3.703738	3.889971	4.552472	5.256426
29	C	2.137488	4.339012	5.022494	3.600173	3.858081
30	O	3.070950	4.138359	4.575627	4.229913	4.724618
31	O	2.828333	5.065849	5.861044	3.721815	3.665469
32	O	4.264635	4.017186	3.888475	5.421595	6.219250
33	C	2.706492	5.016205	5.958355	3.056389	2.755270
34	H	3.795313	5.131754	6.149328	2.763252	2.183375
35	O	2.571504	6.083664	6.978829	4.199442	3.812004

		16	17	18	19	20
16	C	0.000000				
17	H	1.086598	0.000000			
18	C	1.395962	2.155792	0.000000		
19	H	2.156194	2.484044	1.086585	0.000000	
20	C	6.051147	7.072781	5.706110	6.540967	0.000000
21	H	6.488808	7.525416	5.917125	6.632520	1.087797
22	C	6.876629	7.829043	6.718376	7.578590	1.400782
23	H	7.814677	8.755402	7.573369	8.367312	2.158226

This journal is © The Royal Society of Chemistry 2014

24	C	6.759552	7.633805	6.887259	7.832351	2.422913
25	H	7.632271	8.444723	7.840251	8.775082	3.407935
26	C	5.782455	6.631624	6.100668	7.119399	2.809167
27	H	6.062905	6.800767	6.600452	7.638196	3.894787
28	C	5.036359	5.989935	4.682053	5.456434	4.920820
29	C	4.519278	5.301463	4.835015	5.777696	5.572515
30	O	4.796518	5.606635	4.760914	5.554787	5.866445
31	O	4.679412	5.262959	5.273065	6.183587	6.545084
32	O	5.664059	6.596012	5.053145	5.646334	5.437668
33	C	4.455806	5.107599	5.267163	6.334269	4.942021
34	H	4.110446	4.587375	5.119435	6.132641	5.468056
35	O	5.595907	6.213799	6.401262	7.470278	5.537099

		21	22	23	24	25
21	H	0.000000				
22	C	2.164945	0.000000			
23	H	2.491713	1.086720	0.000000		
24	C	3.410526	1.395747	2.156229	0.000000	
25	H	4.309209	2.155801	2.484371	1.086621	0.000000
26	C	3.896933	2.428596	3.412569	1.401657	2.154940
27	H	4.982496	3.406614	4.301005	2.154384	2.470418
28	C	5.072889	6.103593	6.996593	6.373397	7.411811
29	C	6.127213	6.421180	7.462392	6.182592	7.094159
30	O	6.189805	6.925967	7.903068	6.947761	7.936492
31	O	7.183274	7.275083	8.342236	6.855663	7.683554
32	O	5.353092	6.722076	7.513710	7.187746	8.244702
33	C	5.899191	5.156585	6.219414	4.320439	4.957551
34	H	6.429365	5.606299	6.639144	4.708860	5.254405
35	O	6.517316	5.613236	6.635357	4.659655	5.156088

		26	27	28	29	30
26	C	0.000000				
27	H	1.085918	0.000000			
28	C	5.574038	6.167546	0.000000		
29	C	5.007972	5.206445	2.298346	0.000000	
30	O	5.925433	6.303208	1.387456	1.392746	0.000000
31	O	5.567080	5.547647	3.421822	1.197086	2.257794
32	O	6.533766	7.217198	1.199040	3.428398	2.260296
33	C	2.919108	2.587835	4.837212	3.182509	4.470074
34	H	3.362210	2.913539	5.617465	3.956987	5.196599
35	O	3.316371	2.769048	5.275721	3.462281	4.823768

		31	32	33	34	35
31	O	0.000000				
32	O	4.480171	0.000000			
33	C	3.184497	6.007895	0.000000		
34	H	3.795550	6.752262	1.107551	0.000000	
35	O	3.319978	6.470387	1.211298	2.012432	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

This journal is © The Royal Society of Chemistry 2014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.621756	-1.024951	-0.413823
2	6	0	-0.185735	-1.429968	-0.679316
3	1	0	-0.094953	-2.434916	-1.098670
4	6	0	-1.750162	0.267771	0.124283
5	6	0	0.349874	-0.359481	-1.698788
6	1	0	-0.231749	-0.433466	-2.622472
7	6	0	0.585232	-1.265870	0.617907
8	6	0	0.468294	0.013745	1.194806
9	6	0	-0.392508	0.967726	0.357901
10	6	0	0.292895	1.041628	-1.058681
11	1	0	-0.244368	1.776230	-1.666075
12	6	0	1.366016	-2.247129	1.224986
13	1	0	1.459507	-3.229321	0.767699
14	6	0	1.153066	0.306642	2.375206
15	1	0	1.109638	1.295268	2.821719
16	6	0	1.926991	-0.686062	2.989945
17	1	0	2.456189	-0.456983	3.910905
18	6	0	2.032225	-1.956630	2.421357
19	1	0	2.639787	-2.719092	2.901137
20	6	0	-2.751577	-1.792379	-0.684759
21	1	0	-2.645392	-2.789928	-1.105381
22	6	0	-4.022240	-1.271312	-0.408903
23	1	0	-4.907171	-1.868940	-0.610641
24	6	0	-4.151847	0.014658	0.117966
25	1	0	-5.138231	0.421337	0.323887
26	6	0	-3.016425	0.793529	0.380303
27	1	0	-3.137356	1.800066	0.769502
28	6	0	1.815717	-0.564566	-2.043719
29	6	0	1.756077	1.470768	-0.977768
30	8	0	2.558764	0.523288	-1.608416
31	8	0	2.230613	2.446833	-0.472666
32	8	0	2.328178	-1.493856	-2.601842
33	6	0	-0.615854	2.352873	0.952050
34	1	0	-0.598540	2.420040	2.057427
35	8	0	-0.879687	3.327954	0.283581

Rotational constants (GHZ): 0.3746671 0.2672276 0.2547108
Standard basis: 6-31+G(d) (6D, 7F)
There are 461 symmetry adapted basis functions of A symmetry.
Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
461 basis functions, 784 primitive gaussians, 461 cartesian basis functions
79 alpha electrons 79 beta electrons
nuclear repulsion energy 1927.9489791762 Hartrees.

This journal is © The Royal Society of Chemistry 2014

```
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
```

This journal is © The Royal Society of Chemistry 2014

```
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1032.18960837     A.U. after   12 cycles
            Convg  =    0.4849D-08             -V/T =  2.0093
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000020550   -0.000010806    0.000022009
      2        6           0.000000185    0.000042142   -0.000015417
      3        1          -0.000004433    0.000000485   -0.000001999
      4        6          -0.000012582   -0.000016031    0.000006296
      5        6           0.000018632   -0.000111330    0.000028036
      6        1           0.000013331   -0.000002178    0.000000278
      7        6           0.000000644   -0.000002018    0.000001981
      8        6           0.000016033   -0.000042080    0.000040188
      9        6           0.000070359    0.000084039   -0.000097922
     10        6          -0.000040119    0.000045734    0.000058655
     11        1          -0.000006413   -0.000011386   -0.000027018
     12        6           0.000007146   -0.000000819   -0.000000536
     13        1          -0.000000718   -0.000001862   -0.000002445
     14        6          -0.000002540    0.000008254   -0.000005459
     15        1           0.000003673   -0.000000411   -0.000005983
     16        6           0.000001750   -0.000013769   -0.000000890
     17        1           0.000005775   -0.000004088   -0.000002068
     18        6           0.000002322    0.000003375   -0.000004191
     19        1           0.000002025   -0.000002931   -0.000002804
     20        6           0.000002924   -0.000003084    0.000004391
     21        1          -0.000002741    0.000003191   -0.000000995
     22        6          -0.000001923    0.000015775    0.000001656
     23        1          -0.000002948    0.000002729    0.000004137
     24        6          -0.000008507   -0.000012358    0.000005504
     25        1          -0.000001737    0.000001441    0.000005547
     26        6           0.000006012    0.000014168   -0.000001483
     27        1          -0.000003018   -0.000000933    0.000004551
     28        6           0.000004916    0.000269712   -0.000182857
     29        6          -0.000031826    0.000028006    0.000269557
     30        8           0.000007268   -0.000147538   -0.000062493
     31        8          -0.000018209   -0.000013832   -0.000104928
     32        8           0.000008612   -0.000092598    0.000062008
     33        6          -0.000016453   -0.000027754   -0.000027639
     34        1          -0.000012169   -0.000016966    0.000015911
     35        8           0.000015279    0.000015720    0.000016422
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000269712 RMS     0.000052154

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
```

This journal is © The Royal Society of Chemistry 2014

```
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000099263 RMS     0.000018030
 Search for a local minimum.
 Step number   6 out of a maximum of  210
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6
 DE= -5.39D-08 DEPred=-1.14D-06 R= 4.74D-02
 Trust test= 4.74D-02 RLast= 8.39D-03 DXMaxT set to 1.24D-01
     Eigenvalues ---    0.00378   0.00466   0.01077   0.01109
0.01163
     Eigenvalues ---    0.01349   0.01427   0.01497   0.01620
0.01819
     Eigenvalues ---    0.02114   0.02119   0.02130   0.02132
0.02135
     Eigenvalues ---    0.02136   0.02142   0.02145   0.02155
0.02159
     Eigenvalues ---    0.02163   0.02167   0.02727   0.03627
0.03913
     Eigenvalues ---    0.04199   0.04684   0.04905   0.05259
0.05301
     Eigenvalues ---    0.05405   0.05817   0.06323   0.06587
0.08261
     Eigenvalues ---    0.08917   0.09287   0.09995   0.12372
0.15299
     Eigenvalues ---    0.15941   0.15999   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16002   0.16002   0.16018   0.16404
0.20263
     Eigenvalues ---    0.21130   0.21787   0.22000   0.22003
0.22607
     Eigenvalues ---    0.22648   0.22704   0.23765   0.24462
0.24619
     Eigenvalues ---    0.24819   0.24898   0.26106   0.27251
0.27804
     Eigenvalues ---    0.28742   0.28877   0.29427   0.29943
0.30347
     Eigenvalues ---    0.32508   0.34370   0.34417   0.34527
0.35114
     Eigenvalues ---    0.35159   0.35231   0.35244   0.35248
0.35261
     Eigenvalues ---    0.35347   0.35391   0.36715   0.39795
0.41908
     Eigenvalues ---    0.42056   0.42718   0.43402   0.44131
0.45001
     Eigenvalues ---    0.46047   0.46179   0.46317   0.46436
0.46812
```

```
     Eigenvalues ---    0.47741   0.98114   1.04603
1.056311000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     6    5    4    3
2
 RFO step:  Lambda=-2.88971113D-07.
 DIIS coeffs:      0.63352      0.47021     -0.02782     -0.03654
-0.03937
 Iteration  1 RMS(Cart)=  0.00082642 RMS(Int)=  0.00000323
 Iteration  2 RMS(Cart)=  0.00000085 RMS(Int)=  0.00000314
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86384   0.00002   0.00004   0.00002   0.00006
2.86391
    R2        2.65718   0.00000   0.00002  -0.00020  -0.00018
2.65700
    R3        2.63130   0.00000  -0.00003  -0.00012  -0.00014
2.63116
    R4        2.06493   0.00000   0.00000  -0.00002  -0.00002
2.06491
    R5        2.97122  -0.00001  -0.00006  -0.00010  -0.00016
2.97106
    R6        2.86847   0.00002  -0.00010   0.00017   0.00007
2.86854
    R7        2.92006   0.00002   0.00004  -0.00016  -0.00011
2.91995
    R8        2.63574   0.00001   0.00000  -0.00022  -0.00022
2.63552
    R9        2.06746  -0.00001  -0.00001  -0.00001  -0.00003
2.06743
   R10        2.91293   0.00004  -0.00008   0.00025   0.00017
2.91310
   R11        2.87197  -0.00001   0.00003  -0.00021  -0.00019
2.87178
   R12        2.66170  -0.00001  -0.00001  -0.00014  -0.00015
2.66155
   R13        2.63279   0.00001  -0.00002  -0.00010  -0.00013
2.63266
   R14        2.89780   0.00003   0.00004  -0.00005  -0.00001
2.89779
   R15        2.63754  -0.00001   0.00000  -0.00018  -0.00018
2.63736
   R16        2.97711  -0.00007  -0.00011  -0.00065  -0.00076
2.97635
   R17        2.87929  -0.00002  -0.00003  -0.00036  -0.00038
2.87891
   R18        2.06769   0.00001   0.00001  -0.00002   0.00000
2.06769
   R19        2.88554  -0.00001  -0.00009  -0.00008  -0.00016
2.88538
   R20        2.05499   0.00000   0.00000  -0.00004  -0.00005
2.05494
```

This journal is © The Royal Society of Chemistry 2014

R21	2.64530	0.00000	-0.00005	-0.00007	-0.00011
2.64518					
R22	2.05159	0.00000	-0.00003	0.00005	0.00001
2.05160					
R23	2.64718	0.00001	-0.00002	-0.00012	-0.00014
2.64705					
R24	2.05337	0.00000	-0.00001	-0.00002	-0.00003
2.05334					
R25	2.63799	0.00000	-0.00003	-0.00010	-0.00013
2.63785					
R26	2.05335	0.00000	-0.00001	-0.00003	-0.00004
2.05331					
R27	2.05564	0.00000	-0.00001	-0.00005	-0.00005
2.05558					
R28	2.64709	0.00001	-0.00004	-0.00009	-0.00013
2.64697					
R29	2.05360	0.00000	-0.00001	-0.00003	-0.00004
2.05357					
R30	2.63758	-0.00001	-0.00002	-0.00012	-0.00014
2.63744					
R31	2.05342	0.00000	-0.00001	-0.00002	-0.00003
2.05339					
R32	2.64875	0.00001	-0.00003	-0.00010	-0.00013
2.64862					
R33	2.05209	0.00000	-0.00003	0.00004	0.00001
2.05210					
R34	2.62191	-0.00009	0.00010	-0.00046	-0.00036
2.62155					
R35	2.26586	0.00005	-0.00002	0.00002	0.00001
2.26586					
R36	2.63191	0.00010	-0.00006	0.00034	0.00028
2.63219					
R37	2.26216	-0.00006	0.00004	-0.00021	-0.00018
2.26199					
R38	2.09297	0.00001	-0.00003	0.00013	0.00010
2.09307					
R39	2.28902	0.00000	0.00000	0.00000	0.00000
2.28902					
A1	1.98152	0.00000	0.00005	-0.00015	-0.00010
1.98142					
A2	2.19874	0.00001	-0.00005	0.00014	0.00009
2.19882					
A3	2.10257	0.00000	-0.00001	0.00001	0.00001
2.10258					
A4	1.97332	0.00000	0.00007	-0.00012	-0.00005
1.97328					
A5	1.82805	0.00001	0.00004	-0.00010	-0.00007
1.82798					
A6	1.87829	0.00000	0.00007	-0.00011	-0.00004
1.87825					
A7	1.92732	0.00000	-0.00003	-0.00001	-0.00004
1.92728					

This journal is © The Royal Society of Chemistry 2014

A8	1.96622	0.00000	-0.00004	0.00014	0.00011
1.96633					
A9	1.88336	0.00000	-0.00011	0.00019	0.00008
1.88344					
A10	1.97585	0.00000	-0.00007	0.00013	0.00005
1.97591					
A11	2.09405	0.00000	-0.00002	0.00010	0.00009
2.09414					
A12	2.21324	0.00000	0.00009	-0.00023	-0.00014
2.21310					
A13	1.89683	0.00001	-0.00012	0.00018	0.00006
1.89688					
A14	1.91453	-0.00002	-0.00001	-0.00009	-0.00010
1.91443					
A15	1.96476	0.00003	0.00011	0.00010	0.00021
1.96496					
A16	1.97405	0.00001	0.00009	-0.00019	-0.00009
1.97395					
A17	1.88810	-0.00002	0.00003	-0.00008	-0.00005
1.88805					
A18	1.82612	0.00000	-0.00008	0.00007	-0.00001
1.82611					
A19	1.98895	0.00000	0.00000	-0.00003	-0.00003
1.98892					
A20	2.19061	0.00001	-0.00005	0.00015	0.00010
2.19071					
A21	2.10356	-0.00001	0.00006	-0.00012	-0.00006
2.10350					
A22	1.96953	-0.00001	0.00002	-0.00006	-0.00004
1.96949					
A23	2.09014	0.00001	-0.00008	0.00022	0.00014
2.09028					
A24	2.22235	-0.00001	0.00006	-0.00017	-0.00011
2.22224					
A25	1.86912	0.00000	0.00021	-0.00034	-0.00013
1.86899					
A26	1.84165	0.00000	-0.00022	0.00069	0.00047
1.84212					
A27	1.91980	-0.00001	0.00032	-0.00063	-0.00031
1.91949					
A28	1.85012	0.00000	-0.00004	-0.00010	-0.00014
1.84997					
A29	2.02086	-0.00001	0.00011	-0.00031	-0.00020
2.02066					
A30	1.95170	0.00002	-0.00040	0.00077	0.00037
1.95207					
A31	1.92499	0.00002	0.00008	-0.00009	-0.00001
1.92498					
A32	1.98000	-0.00002	-0.00001	0.00003	0.00002
1.98002					
A33	1.81526	-0.00001	0.00015	-0.00033	-0.00018
1.81508					

This journal is © The Royal Society of Chemistry 2014

A34	1.89338	0.00000	-0.00003	0.00026	0.00024
1.89362					
A35	1.96322	-0.00001	-0.00026	-0.00003	-0.00029
1.96293					
A36	1.88730	0.00002	0.00006	0.00014	0.00020
1.88749					
A37	2.09565	0.00000	0.00001	-0.00002	-0.00001
2.09564					
A38	2.08629	0.00000	0.00000	-0.00003	-0.00003
2.08625					
A39	2.10124	0.00000	-0.00001	0.00005	0.00004
2.10128					
A40	2.11684	0.00000	0.00001	-0.00001	0.00000
2.11684					
A41	2.08688	0.00000	0.00004	-0.00013	-0.00010
2.08679					
A42	2.07937	0.00001	-0.00004	0.00013	0.00009
2.07946					
A43	2.08474	0.00000	0.00000	-0.00003	-0.00003
2.08471					
A44	2.10355	0.00000	0.00001	0.00001	0.00002
2.10356					
A45	2.09485	0.00000	-0.00001	0.00002	0.00001
2.09486					
A46	2.09568	0.00000	-0.00002	0.00006	0.00004
2.09572					
A47	2.09193	0.00000	0.00000	-0.00001	-0.00001
2.09192					
A48	2.09552	0.00000	0.00002	-0.00005	-0.00003
2.09549					
A49	2.09607	0.00000	0.00000	0.00002	0.00001
2.09609					
A50	2.08598	0.00000	0.00001	-0.00008	-0.00006
2.08592					
A51	2.10112	0.00000	-0.00001	0.00006	0.00005
2.10118					
A52	2.09156	0.00000	-0.00001	0.00000	-0.00001
2.09156					
A53	2.09589	0.00000	0.00000	0.00003	0.00003
2.09592					
A54	2.09572	0.00000	0.00001	-0.00003	-0.00002
2.09570					
A55	2.09515	0.00000	0.00000	0.00002	0.00002
2.09517					
A56	2.10297	0.00000	0.00001	0.00002	0.00003
2.10299					
A57	2.08506	0.00000	0.00000	-0.00004	-0.00004
2.08502					
A58	2.08473	0.00000	0.00000	-0.00008	-0.00008
2.08465					
A59	2.11330	0.00001	0.00002	-0.00002	0.00000
2.11330					

A60	2.08510	0.00000	-0.00002	0.00010	0.00008	2.08518
A61	1.91721	0.00002	-0.00001	0.00011	0.00009	1.91731
A62	2.24267	-0.00004	0.00003	-0.00027	-0.00025	2.24242
A63	2.12330	0.00002	0.00000	0.00015	0.00014	2.12345
A64	1.91461	-0.00002	-0.00007	0.00010	0.00002	1.91462
A65	2.25411	0.00003	-0.00007	0.00016	0.00008	2.25419
A66	2.11447	-0.00001	0.00018	-0.00026	-0.00010	2.11438
A67	1.94637	0.00000	0.00004	-0.00012	-0.00008	1.94629
A68	2.02865	-0.00003	0.00014	-0.00056	-0.00044	2.02821
A69	2.15141	0.00004	-0.00017	0.00033	0.00013	2.15155
A70	2.10060	-0.00001	0.00007	0.00023	0.00027	2.10088
D1	-3.14006	0.00000	0.00017	0.00002	0.00019	-3.13987
D2	-1.04074	0.00000	0.00019	-0.00012	0.00007	-1.04067
D3	0.96036	0.00001	0.00012	0.00000	0.00012	0.96048
D4	-0.02734	0.00000	0.00005	-0.00004	0.00002	-0.02733
D5	2.07198	0.00000	0.00008	-0.00018	-0.00010	2.07188
D6	-2.21010	0.00001	0.00000	-0.00006	-0.00006	-2.21016
D7	-0.02689	0.00000	-0.00026	0.00018	-0.00008	-0.02696
D8	3.10557	0.00000	-0.00018	-0.00013	-0.00031	3.10526
D9	-3.14137	0.00000	-0.00014	0.00023	0.00009	-3.14129
D10	-0.00892	0.00000	-0.00007	-0.00007	-0.00014	-0.00906
D11	0.02570	0.00000	0.00009	0.00000	0.00010	0.02580
D12	-3.11841	0.00000	0.00012	0.00013	0.00025	-3.11816
D13	3.13659	0.00000	-0.00003	-0.00006	-0.00010	3.13649
D14	-0.00753	0.00000	0.00000	0.00006	0.00006	-0.00747
D15	-1.09547	0.00000	-0.00029	0.00109	0.00080	-1.09467

This journal is © The Royal Society of Chemistry 2014

D16	1.07091	0.00000	-0.00027	0.00091	0.00065	1.07156
D17	3.09652	0.00000	-0.00031	0.00101	0.00070	3.09722
D18	1.03421	0.00000	-0.00020	0.00087	0.00068	1.03489
D19	-3.08260	0.00000	-0.00017	0.00070	0.00053	-3.08207
D20	-1.05699	0.00000	-0.00022	0.00080	0.00058	-1.05641
D21	-3.09302	-0.00001	-0.00034	0.00117	0.00084	-3.09218
D22	-0.92664	-0.00001	-0.00031	0.00100	0.00069	-0.92595
D23	1.09897	0.00000	-0.00036	0.00110	0.00074	1.09971
D24	-0.93654	0.00000	0.00000	0.00012	0.00012	-0.93642
D25	2.21693	-0.00001	0.00004	-0.00004	0.00000	2.21693
D26	-3.12354	0.00000	-0.00011	0.00025	0.00014	-3.12341
D27	0.02992	0.00000	-0.00008	0.00010	0.00002	0.02994
D28	1.02747	0.00000	0.00003	0.00004	0.00007	1.02754
D29	-2.10225	0.00000	0.00006	-0.00012	-0.00006	-2.10230
D30	-0.92291	0.00000	0.00033	-0.00046	-0.00013	-0.92304
D31	1.04282	0.00000	0.00028	-0.00042	-0.00014	1.04268
D32	-3.13249	0.00002	-0.00016	0.00057	0.00041	-3.13208
D33	2.22857	0.00000	0.00025	-0.00013	0.00011	2.22869
D34	-2.08889	0.00000	0.00019	-0.00009	0.00011	-2.08878
D35	0.01899	0.00002	-0.00024	0.00090	0.00066	0.01965
D36	0.01873	0.00000	0.00011	-0.00001	0.00010	0.01883
D37	-3.11137	0.00000	0.00006	0.00009	0.00015	-3.11122
D38	-3.13336	0.00000	0.00020	-0.00036	-0.00016	-3.13352
D39	0.01973	0.00000	0.00014	-0.00026	-0.00011	0.01962
D40	-0.08259	0.00000	0.00035	-0.00139	-0.00104	-0.08363
D41	-2.21056	0.00000	0.00033	-0.00169	-0.00135	-2.21192

This journal is © The Royal Society of Chemistry 2014

D42	2.02627	-0.00001	0.00017	-0.00166	-0.00149	2.02478
D43	2.03806	0.00000	0.00024	-0.00135	-0.00110	2.03695
D44	-0.08991	0.00000	0.00023	-0.00165	-0.00142	-0.09133
D45	-2.13627	-0.00001	0.00006	-0.00162	-0.00156	-2.13782
D46	-2.19415	-0.00002	0.00027	-0.00150	-0.00122	-2.19537
D47	1.96107	-0.00003	0.00026	-0.00180	-0.00154	1.95953
D48	-0.08528	-0.00003	0.00009	-0.00177	-0.00167	-0.08696
D49	-2.02683	0.00004	-0.00008	0.00168	0.00159	-2.02524
D50	1.11334	-0.00003	-0.00107	-0.00046	-0.00153	1.11181
D51	2.16011	0.00003	-0.00002	0.00145	0.00143	2.16155
D52	-0.98290	-0.00005	-0.00100	-0.00069	-0.00169	-0.98459
D53	0.05112	0.00003	-0.00009	0.00167	0.00158	0.05270
D54	-3.09189	-0.00005	-0.00108	-0.00047	-0.00155	-3.09344
D55	-0.02294	0.00000	0.00010	-0.00044	-0.00034	-0.02328
D56	-3.11650	0.00000	0.00018	-0.00015	0.00003	-3.11647
D57	3.10744	0.00000	0.00007	-0.00030	-0.00023	3.10721
D58	0.01387	0.00000	0.00015	0.00000	0.00014	0.01402
D59	-0.00139	0.00000	-0.00006	0.00006	0.00000	-0.00139
D60	3.13477	0.00000	0.00004	-0.00004	0.00000	3.13477
D61	-3.13039	0.00000	-0.00002	-0.00010	-0.00013	-3.13052
D62	0.00577	0.00000	0.00008	-0.00021	-0.00013	0.00564
D63	0.94687	0.00000	-0.00019	0.00055	0.00035	0.94722
D64	-1.01308	0.00000	-0.00002	-0.00004	-0.00006	-1.01314
D65	3.09512	-0.00002	0.00046	-0.00075	-0.00029	3.09483
D66	-2.24717	0.00000	-0.00028	0.00024	-0.00004	-2.24721
D67	2.07607	0.00000	-0.00011	-0.00034	-0.00045	2.07562

This journal is © The Royal Society of Chemistry 2014

D68	-0.09891	-0.00002	0.00037	-0.00106	-0.00069	-0.09960
D69	3.10230	0.00000	-0.00004	-0.00022	-0.00026	3.10204
D70	-0.02438	0.00000	-0.00029	0.00024	-0.00005	-0.02443
D71	0.01638	0.00000	0.00005	0.00012	0.00017	0.01654
D72	-3.11030	0.00000	-0.00020	0.00057	0.00037	-3.10993
D73	-0.93750	0.00000	-0.00037	0.00122	0.00085	-0.93665
D74	1.24089	-0.00001	-0.00035	0.00138	0.00103	1.24192
D75	-2.95537	0.00001	-0.00045	0.00171	0.00125	-2.95412
D76	1.04152	0.00000	-0.00025	0.00109	0.00084	1.04236
D77	-3.06328	-0.00001	-0.00023	0.00125	0.00102	-3.06225
D78	-0.97636	0.00000	-0.00033	0.00158	0.00125	-0.97511
D79	-3.02440	0.00000	-0.00041	0.00113	0.00073	-3.02367
D80	-0.84602	-0.00001	-0.00038	0.00129	0.00091	-0.84511
D81	1.24090	0.00001	-0.00049	0.00162	0.00113	1.24204
D82	1.61938	-0.00002	-0.00034	-0.00290	-0.00324	1.61615
D83	-1.44607	-0.00002	0.00006	-0.00285	-0.00280	-1.44887
D84	-0.50199	0.00000	-0.00095	-0.00172	-0.00267	-0.50466
D85	2.71574	0.00000	-0.00055	-0.00168	-0.00223	2.71351
D86	-2.62352	-0.00001	-0.00065	-0.00197	-0.00263	-2.62614
D87	0.59421	-0.00001	-0.00025	-0.00193	-0.00218	0.59203
D88	0.09600	0.00002	-0.00007	0.00139	0.00131	0.09731
D89	-3.04440	-0.00004	-0.00118	-0.00017	-0.00135	-3.04575
D90	2.17902	0.00004	-0.00002	0.00106	0.00104	2.18006
D91	-0.96138	-0.00003	-0.00113	-0.00050	-0.00162	-0.96300
D92	-2.01371	0.00004	-0.00017	0.00146	0.00129	-2.01242
D93	1.12907	-0.00003	-0.00128	-0.00010	-0.00137	1.12770

This journal is © The Royal Society of Chemistry 2014

D94	-0.01474	0.00000	-0.00015	0.00018	0.00003	-0.01471
D95	3.13789	0.00000	-0.00005	-0.00004	-0.00009	3.13779
D96	3.12141	0.00000	-0.00005	0.00008	0.00003	3.12143
D97	-0.00915	0.00000	0.00005	-0.00015	-0.00010	-0.00925
D98	-3.13751	0.00000	0.00019	-0.00018	0.00001	-3.13750
D99	0.01555	0.00000	0.00022	-0.00027	-0.00005	0.01550
D100	0.01868	0.00000	-0.00006	0.00027	0.00021	0.01889
D101	-3.11145	0.00000	-0.00003	0.00018	0.00015	-3.11130
D102	0.00413	0.00000	0.00001	0.00005	0.00006	0.00419
D103	3.13466	0.00000	-0.00009	0.00028	0.00019	3.13485
D104	-3.12593	0.00000	0.00004	-0.00004	0.00000	-3.12593
D105	0.00460	0.00000	-0.00007	0.00019	0.00013	0.00472
D106	-3.13277	0.00000	-0.00006	0.00010	0.00004	-3.13274
D107	0.01401	0.00000	0.00003	0.00004	0.00007	0.01408
D108	0.00629	0.00000	-0.00003	0.00022	0.00019	0.00648
D109	-3.13011	0.00000	0.00006	0.00016	0.00022	-3.12989
D110	3.13263	0.00000	-0.00005	0.00002	-0.00003	3.13260
D111	-0.00413	0.00000	0.00001	-0.00012	-0.00011	-0.00424
D112	-0.00376	0.00000	0.00005	-0.00004	0.00000	-0.00376
D113	-3.14052	0.00000	0.00010	-0.00018	-0.00008	-3.14060
D114	-0.01230	0.00000	-0.00008	0.00011	0.00003	-0.01227
D115	3.11799	0.00000	-0.00003	0.00001	-0.00002	3.11797
D116	3.13410	0.00000	-0.00002	-0.00003	-0.00005	3.13405
D117	-0.01880	0.00000	0.00003	-0.00013	-0.00010	-0.01890
D118	0.00965	-0.00002	0.00004	-0.00084	-0.00079	0.00886
D119	-3.13064	0.00005	0.00095	0.00113	0.00208	-3.12856

```
   D120       -0.06851  -0.00001   0.00003  -0.00040  -0.00037  -
0.06888
   D121        3.07200   0.00006   0.00102   0.00102   0.00204
3.07404
         Item               Value     Threshold  Converged?
 Maximum Force            0.000099     0.000450     YES
 RMS     Force            0.000018     0.000300     YES
 Maximum Displacement     0.006617     0.001800     NO
 RMS     Displacement     0.000826     0.001200     YES
 Predicted change in Energy=-8.726749D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.620162   -1.034015   -0.392974
      2          6           0       -0.184854   -1.436140   -0.666780
      3          1           0       -0.093777   -2.444799   -1.077035
      4          6           0       -1.748895    0.263446    0.133263
      5          6           0        0.337690   -0.373794   -1.701304
      6          1           0       -0.252046   -0.458596   -2.618878
      7          6           0        0.596485   -1.256244    0.622160
      8          6           0        0.479288    0.028455    1.187401
      9          6           0       -0.392071    0.970806    0.348261
     10          6           0        0.281460    1.033271   -1.074106
     11          1           0       -0.262733    1.760468   -1.684231
     12          6           0        1.386243   -2.228304    1.232267
     13          1           0        1.479755   -3.214612    0.783992
     14          6           0        1.172794    0.335858    2.358868
     15          1           0        1.129266    1.328775    2.795764
     16          6           0        1.955879   -0.647583    2.976722
     17          1           0        2.491937   -0.407268    3.890806
     18          6           0        2.061360   -1.923264    2.419922
     19          1           0        2.675918   -2.678526    2.902131
     20          6           0       -2.749256   -1.808251   -0.646633
     21          1           0       -2.642873   -2.809495   -1.058256
     22          6           0       -4.019412   -1.289086   -0.365248
     23          1           0       -4.903766   -1.891928   -0.553444
     24          6           0       -4.149378    0.001588    0.149695
     25          1           0       -5.135484    0.406725    0.359864
     26          6           0       -3.014780    0.787171    0.394637
     27          1           0       -3.136134    1.797160    0.774671
     28          6           0        1.800952   -0.576915   -2.057735
     29          6           0        1.743934    1.467132   -1.008661
     30          8           0        2.544288    0.516610   -1.638023
     31          8           0        2.219549    2.449772   -0.517742
     32          8           0        2.311635   -1.510453   -2.610376
     33          6           0       -0.616114    2.360487    0.930927
```

34	1	0	-0.592677	2.437334	2.035614
35	8	0	-0.887028	3.328650	0.255275

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515515	0.000000			
3	H	2.188173	1.092702	0.000000		
4	C	1.406023	2.444358	3.396885	0.000000	
5	C	2.445569	1.572219	2.205661	2.850535	0.000000
6	H	2.675351	2.184216	2.519391	3.214994	1.094039
7	C	2.448144	1.517965	2.185495	2.837127	2.498836
8	C	2.834452	2.454406	3.401920	2.476132	2.920013
9	C	2.465145	2.620426	3.713058	1.545171	2.557581
10	C	2.890291	2.545851	3.498254	2.484494	1.541549
11	H	3.364386	3.355529	4.252235	2.784427	2.217177
12	C	3.620249	2.588869	2.751400	4.152796	3.625535
13	H	3.968594	2.835246	2.555785	4.790044	3.943508
14	C	4.153286	3.760017	4.598009	3.673531	4.205473
15	H	4.828062	4.621783	5.543849	4.062961	4.873290
16	C	4.928717	4.298798	4.885082	4.758213	4.957563
17	H	5.971008	5.384735	5.959605	5.705580	5.992795
18	C	4.717706	3.848440	4.140691	4.952631	4.728256
19	H	5.658484	4.739690	4.853824	5.991728	5.654265
20	C	1.392350	2.591338	2.764418	2.429174	3.563599
21	H	2.154267	2.842748	2.575120	3.414949	3.902551
22	C	2.412929	3.849205	4.153663	2.795374	4.648349
23	H	3.397620	4.742228	4.869888	3.882063	5.576305
24	C	2.786377	4.295480	4.892604	2.414778	4.868356
25	H	3.872981	5.381346	5.967803	3.397184	5.900276
26	C	2.425285	3.752093	4.598229	1.394657	4.120664
27	H	3.417179	4.608911	5.538859	2.165205	4.786538
28	C	3.832022	2.572246	2.835624	4.255360	1.519682
29	C	4.236974	3.502298	4.322622	3.866873	2.417909
30	O	4.614892	3.493531	4.005501	4.651126	2.380315
31	O	5.186108	4.572054	5.442528	4.577377	3.593708
32	O	4.539041	3.164735	3.001690	5.211735	2.452522
33	C	3.779348	4.141622	5.234073	2.513373	3.913398
34	H	4.359361	4.740575	5.811429	3.111522	4.767870
35	O	4.471080	4.903719	5.978044	3.186405	4.363052

		6	7	8	9	10
6	H	0.000000				
7	C	3.443919	0.000000			
8	C	3.906383	1.408433	0.000000		
9	C	3.296470	2.451941	1.533443	0.000000	
10	C	2.212830	2.866782	2.482580	1.575016	0.000000
11	H	2.407888	3.893359	3.434637	2.184335	1.094173
12	C	4.543916	1.393143	2.432600	3.765390	4.144607
13	H	4.708958	2.154428	3.417771	4.605574	4.788836
14	C	5.238252	2.425505	1.395630	2.625738	3.614717
15	H	5.866947	3.419171	2.167979	2.903942	3.972656
16	C	6.018421	2.786106	2.416406	3.878255	4.694482

This journal is © The Royal Society of Chemistry 2014

17	H	7.064564	3.872666	3.398383	4.771395	5.622429
18	C	5.734685	2.413032	2.798440	4.322817	4.910945
19	H	6.631939	3.397822	3.885001	5.408552	5.943175
20	C	3.456499	3.620571	4.142544	3.777471	4.176389
21	H	3.698421	3.966084	4.779626	4.618990	4.828956
22	C	4.467842	4.720440	4.938110	4.332875	4.938959
23	H	5.287624	5.660292	5.974587	5.418829	5.976156
24	C	4.802704	4.932401	4.743638	3.885378	4.711091
25	H	5.785297	5.974088	5.688020	4.776849	5.638449
26	C	4.273864	4.155544	3.662327	2.629539	3.617039
27	H	4.992251	4.824829	4.045978	2.897338	3.959980
28	C	2.131591	3.015637	3.555865	3.604664	2.422618
29	C	3.207049	3.375351	2.914071	2.578778	1.526875
30	O	3.119710	3.470645	3.533488	3.574049	2.388584
31	O	4.356852	4.203363	3.434937	3.123758	2.464184
32	O	2.771089	3.668195	4.488746	4.713831	3.598926
33	C	4.547626	3.827072	2.589220	1.523454	2.566574
34	H	5.492426	4.129706	2.769706	2.244573	3.522196
35	O	4.796581	4.832873	3.691471	2.411028	2.898513

		11	12	13	14	15
11	H	0.000000				
12	C	5.209163	0.000000			
13	H	5.820636	1.087428	0.000000		
14	C	4.520720	2.808864	3.896190	0.000000	
15	H	4.711091	3.894017	4.981208	1.085660	0.000000
16	C	5.696090	2.422042	3.409457	1.400758	2.149890
17	H	6.585463	3.406840	4.307898	2.153881	2.463703
18	C	5.984594	1.399771	2.163819	2.428355	3.403794
19	H	7.026739	2.157408	2.490925	3.411895	4.296732
20	C	4.471595	4.561695	4.680713	5.386345	6.060855
21	H	5.190517	4.670979	4.533658	6.010765	6.797630
22	C	5.015190	5.714480	5.938791	6.084427	6.584381
23	H	6.013141	6.547222	6.654891	7.097124	7.614959
24	C	4.643592	6.065268	6.514093	5.772148	6.052040
25	H	5.454782	7.087833	7.553499	6.617810	6.784606
26	C	3.583680	5.400344	6.030482	4.647329	4.819944
27	H	3.782060	6.071708	6.813543	4.817877	4.743188
28	C	3.140328	3.704481	3.890504	4.553474	5.257306
29	C	2.137558	4.336582	5.020171	3.598088	3.856243
30	O	3.070617	4.136929	4.573992	4.229516	4.724443
31	O	2.827996	5.063726	5.858928	3.720110	3.663969
32	O	4.264275	4.017159	3.888176	5.422104	6.219772
33	C	2.706281	5.015700	5.957851	3.055869	2.754705
34	H	3.795295	5.131243	6.148660	2.763617	2.184448
35	O	2.571113	6.082927	6.978214	4.198187	3.810383

		16	17	18	19	20
16	C	0.000000				
17	H	1.086581	0.000000			
18	C	1.395892	2.155722	0.000000		
19	H	2.156096	2.483936	1.086567	0.000000	
20	C	6.050963	7.072567	5.706051	6.540919	0.000000
21	H	6.488716	7.525302	5.917173	6.632598	1.087769

This journal is © The Royal Society of Chemistry 2014

22	C	6.876365	7.828745	6.718269	7.578506	1.400716
23	H	7.814423	8.755112	7.573300	8.367278	2.158147
24	C	6.759265	7.633487	6.887107	7.832214	2.422807
25	H	7.631968	8.444387	7.840105	8.774958	3.407820
26	C	5.782139	6.631275	6.100446	7.119173	2.809086
27	H	6.062540	6.800366	6.600178	7.637918	3.894710
28	C	5.037336	5.990941	4.682935	5.457344	4.920548
29	C	4.516660	5.298835	4.832259	5.774891	5.572069
30	O	4.795565	5.605732	4.759530	5.553307	5.865957
31	O	4.677008	5.260433	5.270516	6.180877	6.544952
32	O	5.664519	6.596582	5.053410	5.646666	5.436690
33	C	4.455212	5.106988	5.266546	6.333623	4.941393
34	H	4.110661	4.587846	5.119220	6.132420	5.465370
35	O	5.594535	6.212211	6.400101	7.469042	5.537967

		21	22	23	24	25
21	H	0.000000				
22	C	2.164893	0.000000			
23	H	2.491667	1.086701	0.000000		
24	C	3.410409	1.395671	2.156133	0.000000	
25	H	4.309089	2.155732	2.484277	1.086606	0.000000
26	C	3.896822	2.428488	3.412433	1.401588	2.154839
27	H	4.982388	3.406539	4.300904	2.154376	2.470379
28	C	5.072568	6.103141	6.996098	6.372898	7.411239
29	C	6.126668	6.420815	7.462065	6.182292	7.093921
30	O	6.189163	6.925507	7.902587	6.947399	7.936153
31	O	7.182979	7.275090	8.342257	6.855822	7.683797
32	O	5.351984	6.720994	7.512557	7.186720	8.243633
33	C	5.898586	5.155763	6.218549	4.319569	4.956612
34	H	6.426861	5.602933	6.635602	4.705281	5.250582
35	O	6.518065	5.614300	6.636463	4.660838	5.157321

		26	27	28	29	30
26	C	0.000000				
27	H	1.085923	0.000000			
28	C	5.573700	6.167136	0.000000		
29	C	5.007689	5.206174	2.298245	0.000000	
30	O	5.925213	6.303022	1.387265	1.392894	0.000000
31	O	5.567304	5.547934	3.421642	1.196993	2.257786
32	O	6.532984	7.216441	1.199043	3.428379	2.260217
33	C	2.918309	2.586939	4.837628	3.182753	4.470742
34	H	3.358932	2.910150	5.618777	3.958365	5.198590
35	O	3.317509	2.770146	5.275290	3.461899	4.823492

		31	32	33	34	35
31	O	0.000000				
32	O	4.480064	0.000000			
33	C	3.185530	6.008055	0.000000		
34	H	3.798473	6.753168	1.107605	0.000000	
35	O	3.319759	6.469955	1.211296	2.012634	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1

This journal is © The Royal Society of Chemistry 2014

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.621927	-1.025982	-0.410748
2	6	0	-0.185894	-1.431630	-0.675406
3	1	0	-0.095171	-2.437698	-1.092052
4	6	0	-1.750193	0.268201	0.123612
5	6	0	0.349289	-0.363984	-1.697944
6	1	0	-0.233049	-0.440034	-2.620994
7	6	0	0.585283	-1.263850	0.621265
8	6	0	0.468177	0.017252	1.194632
9	6	0	-0.392572	0.968839	0.354967
10	6	0	0.293087	1.038808	-1.061243
11	1	0	-0.243237	1.772379	-1.670704
12	6	0	1.366243	-2.243212	1.231017
13	1	0	1.459805	-3.226670	0.776533
14	6	0	1.152989	0.313701	2.374011
15	1	0	1.109529	1.303658	2.817581
16	6	0	1.927169	-0.677071	2.991374
17	1	0	2.456444	-0.445283	3.911591
18	6	0	2.032522	-1.949170	2.426413
19	1	0	2.640176	-2.710167	2.908354
20	6	0	-2.751755	-1.794089	-0.679334
21	1	0	-2.645685	-2.792790	-1.097168
22	6	0	-4.022266	-1.272088	-0.404886
23	1	0	-4.907269	-1.870204	-0.604748
24	6	0	-4.151696	0.015393	0.118123
25	1	0	-5.138000	0.422790	0.322923
26	6	0	-3.016249	0.794887	0.378120
27	1	0	-3.136990	1.802614	0.764302
28	6	0	1.814713	-0.570155	-2.043572
29	6	0	1.756581	1.466612	-0.980495
30	8	0	2.558607	0.517525	-1.609894
31	8	0	2.231751	2.443928	-0.478640
32	8	0	2.326502	-1.501697	-2.598555
33	6	0	-0.616271	2.355204	0.945613
34	1	0	-0.601806	2.424133	2.050976
35	8	0	-0.877874	3.329154	0.274626

Rotational constants (GHZ): 0.3747392 0.2672407 0.2547577

Standard basis: 6-31+G(d) (6D, 7F)

There are 461 symmetry adapted basis functions of A symmetry.

Integral buffers will be 262144 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

461 basis functions, 784 primitive gaussians, 461 cartesian basis functions

79 alpha electrons 79 beta electrons

```
      nuclear repulsion energy      1928.0683915990 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
```

This journal is © The Royal Society of Chemistry 2014

```
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1032.18960797     A.U. after   12 cycles
            Convg  =    0.6104D-08             -V/T =  2.0093
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000062981   -0.000034534    0.000003523
      2        6           0.000001826    0.000008893   -0.000003052
      3        1           0.000002262   -0.000009338    0.000007081
      4        6           0.000041743    0.000028915   -0.000014713
      5        6          -0.000047010    0.000021048   -0.000094719
      6        1          -0.000017421   -0.000007294    0.000004972
      7        6          -0.000039571   -0.000027521   -0.000044718
      8        6          -0.000018876   -0.000000183    0.000003707
      9        6           0.000041116    0.000020744    0.000014654
     10        6          -0.000016719   -0.000069806    0.000052922
     11        1           0.000022766    0.000002524   -0.000039865
     12        6           0.000010550   -0.000039613   -0.000023405
     13        1           0.000005438   -0.000017538   -0.000007825
     14        6           0.000009201    0.000052070    0.000018206
     15        1          -0.000000476   -0.000004189   -0.000004269
     16        6           0.000025185    0.000003957    0.000059767
     17        1           0.000015583   -0.000004849    0.000009335
     18        6           0.000024679   -0.000043622    0.000020945
     19        1           0.000014915   -0.000011871   -0.000001081
     20        6           0.000014319   -0.000037076   -0.000016859
     21        1          -0.000004522   -0.000017105   -0.000004341
     22        6          -0.000049113   -0.000018425   -0.000009477
     23        1          -0.000014887   -0.000004606   -0.000000821
     24        6          -0.000074567    0.000019225    0.000032350
     25        1          -0.000015608    0.000001438    0.000003898
     26        6          -0.000029044    0.000062901    0.000016019
     27        1          -0.000012989   -0.000003920    0.000006436
     28        6           0.000036049    0.000035512    0.000172698
     29        6          -0.000038858    0.000137630   -0.000121147
     30        8           0.000005719   -0.000068890   -0.000045220
     31        8           0.000045210    0.000025055    0.000062767
     32        8           0.000025506   -0.000057680   -0.000100059
     33        6          -0.000041545    0.000005031    0.000004515
     34        1          -0.000008580    0.000020969   -0.000003799
     35        8           0.000024737    0.000032150    0.000041577
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000172698 RMS     0.000040166
```

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000124059 RMS     0.000025968
 Search for a local minimum.
 Step number   7 out of a maximum of  210
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7
 DE=  3.98D-07 DEPred=-8.73D-07 R=-4.56D-01
 Trust test=-4.56D-01 RLast= 1.06D-02 DXMaxT set to 6.21D-02
     Eigenvalues ---    0.00290   0.00479   0.01065   0.01117
0.01162
     Eigenvalues ---    0.01427   0.01479   0.01594   0.01804
0.01930
     Eigenvalues ---    0.02115   0.02120   0.02130   0.02132
0.02134
     Eigenvalues ---    0.02137   0.02141   0.02145   0.02156
0.02159
     Eigenvalues ---    0.02165   0.02168   0.02766   0.03852
0.03877
     Eigenvalues ---    0.04489   0.04785   0.04937   0.05213
0.05309
     Eigenvalues ---    0.05396   0.05844   0.06199   0.06578
0.08318
     Eigenvalues ---    0.09015   0.09399   0.09948   0.12395
0.15300
     Eigenvalues ---    0.15928   0.15999   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16002   0.16002   0.16048   0.16514
0.20308
     Eigenvalues ---    0.20920   0.21650   0.22000   0.22002
0.22610
     Eigenvalues ---    0.22678   0.22960   0.23750   0.24350
0.24629
     Eigenvalues ---    0.24684   0.24896   0.26123   0.27346
0.28009
     Eigenvalues ---    0.28740   0.28826   0.29470   0.29966
0.31267
     Eigenvalues ---    0.32477   0.34369   0.34416   0.34528
0.35129
     Eigenvalues ---    0.35168   0.35234   0.35244   0.35248
0.35322
     Eigenvalues ---    0.35345   0.35382   0.36712   0.39967
0.41995
     Eigenvalues ---    0.42089   0.42455   0.43554   0.44187
0.44905
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.46049   0.46177   0.46302   0.46444
0.46812
     Eigenvalues ---    0.50683   0.97734   1.04850
1.055071000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     7    6    5    4
3
 RFO step:  Lambda=-2.74222031D-07.
 DIIS coeffs:      0.65767      0.30135      0.03580      0.00315
0.00203
 Iteration  1 RMS(Cart)=  0.00055075 RMS(Int)=  0.00000064
 Iteration  2 RMS(Cart)=  0.00000062 RMS(Int)=  0.00000025
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86391   0.00001  -0.00003   0.00010   0.00007
2.86398
    R2        2.65700   0.00007   0.00008   0.00000   0.00008
2.65708
    R3        2.63116   0.00007   0.00007   0.00002   0.00008
2.63124
    R4        2.06491   0.00001   0.00001   0.00000   0.00001
2.06492
    R5        2.97106   0.00003   0.00007  -0.00006   0.00001
2.97108
    R6        2.86854   0.00001  -0.00002   0.00000  -0.00003
2.86851
    R7        2.91995   0.00006   0.00006   0.00012   0.00018
2.92013
    R8        2.63552   0.00012   0.00010   0.00005   0.00015
2.63567
    R9        2.06743   0.00000   0.00001  -0.00001   0.00001
2.06744
   R10        2.91310   0.00004  -0.00005   0.00024   0.00018
2.91329
   R11        2.87178   0.00004   0.00007  -0.00008  -0.00001
2.87177
   R12        2.66155   0.00007   0.00006  -0.00002   0.00004
2.66160
   R13        2.63266   0.00007   0.00006   0.00003   0.00009
2.63275
   R14        2.89779   0.00007   0.00002   0.00024   0.00026
2.89804
   R15        2.63736   0.00007   0.00008   0.00000   0.00008
2.63744
   R16        2.97635   0.00009   0.00032  -0.00035  -0.00003
2.97632
   R17        2.87891   0.00007   0.00016  -0.00013   0.00003
2.87894
   R18        2.06769   0.00001   0.00001   0.00004   0.00005
2.06773
   R19        2.88538   0.00006   0.00007  -0.00001   0.00006
2.88544
```

This journal is © The Royal Society of Chemistry 2014

R20	2.05494	0.00002	0.00002	0.00001	0.00003
2.05497					
R21	2.64518	0.00006	0.00006	0.00002	0.00008
2.64526					
R22	2.05160	0.00000	0.00000	0.00000	0.00000
2.05160					
R23	2.64705	0.00008	0.00007	0.00004	0.00011
2.64716					
R24	2.05334	0.00002	0.00002	0.00001	0.00003
2.05337					
R25	2.63785	0.00006	0.00006	0.00002	0.00008
2.63794					
R26	2.05331	0.00002	0.00002	0.00001	0.00002
2.05334					
R27	2.05558	0.00002	0.00002	0.00000	0.00003
2.05561					
R28	2.64697	0.00008	0.00006	0.00004	0.00011
2.64708					
R29	2.05357	0.00002	0.00002	0.00001	0.00002
2.05359					
R30	2.63744	0.00006	0.00007	0.00000	0.00007
2.63750					
R31	2.05339	0.00001	0.00001	0.00001	0.00002
2.05341					
R32	2.64862	0.00008	0.00006	0.00005	0.00012
2.64873					
R33	2.05210	0.00000	0.00000	0.00001	0.00000
2.05210					
R34	2.62155	-0.00002	0.00014	-0.00027	-0.00014
2.62141					
R35	2.26586	0.00010	0.00001	0.00011	0.00011
2.26598					
R36	2.63219	0.00007	-0.00010	0.00034	0.00024
2.63243					
R37	2.26199	0.00006	0.00007	-0.00006	0.00001
2.26200					
R38	2.09307	0.00000	-0.00005	0.00002	-0.00002
2.09305					
R39	2.28902	0.00000	0.00001	0.00003	0.00004
2.28906					
A1	1.98142	0.00001	0.00004	-0.00001	0.00003
1.98145					
A2	2.19882	-0.00001	-0.00004	0.00001	-0.00003
2.19879					
A3	2.10258	0.00000	0.00000	0.00000	0.00000
2.10258					
A4	1.97328	0.00000	0.00001	-0.00005	-0.00004
1.97324					
A5	1.82798	-0.00001	0.00001	0.00003	0.00005
1.82803					
A6	1.87825	0.00001	0.00001	-0.00004	-0.00003
1.87821					

This journal is © The Royal Society of Chemistry 2014

A7	1.92728	0.00000	0.00002	0.00000	0.00003
1.92731					
A8	1.96633	-0.00001	-0.00004	-0.00003	-0.00008
1.96625					
A9	1.88344	0.00002	-0.00001	0.00010	0.00009
1.88353					
A10	1.97591	-0.00002	-0.00002	-0.00002	-0.00004
1.97586					
A11	2.09414	-0.00002	-0.00004	0.00001	-0.00003
2.09411					
A12	2.21310	0.00004	0.00006	0.00001	0.00007
2.21317					
A13	1.89688	-0.00001	-0.00003	-0.00007	-0.00010
1.89678					
A14	1.91443	0.00001	0.00004	-0.00007	-0.00003
1.91440					
A15	1.96496	-0.00001	-0.00005	0.00015	0.00010
1.96506					
A16	1.97395	0.00000	0.00004	-0.00003	0.00001
1.97397					
A17	1.88805	0.00001	0.00000	0.00007	0.00007
1.88812					
A18	1.82611	-0.00001	0.00000	-0.00004	-0.00004
1.82607					
A19	1.98892	0.00000	0.00001	-0.00004	-0.00003
1.98889					
A20	2.19071	0.00000	-0.00004	0.00006	0.00002
2.19073					
A21	2.10350	0.00000	0.00002	-0.00001	0.00001
2.10351					
A22	1.96949	-0.00001	0.00002	0.00002	0.00003
1.96952					
A23	2.09028	-0.00001	-0.00005	0.00003	-0.00002
2.09026					
A24	2.22224	0.00002	0.00004	-0.00006	-0.00002
2.22223					
A25	1.86899	0.00000	0.00004	-0.00012	-0.00008
1.86891					
A26	1.84212	-0.00001	-0.00018	0.00005	-0.00012
1.84200					
A27	1.91949	0.00000	0.00011	-0.00022	-0.00011
1.91938					
A28	1.84997	0.00000	0.00005	0.00007	0.00012
1.85010					
A29	2.02066	0.00000	0.00007	-0.00022	-0.00016
2.02050					
A30	1.95207	0.00002	-0.00011	0.00045	0.00034
1.95241					
A31	1.92498	-0.00001	0.00000	0.00003	0.00003
1.92501					
A32	1.98002	-0.00001	-0.00003	-0.00031	-0.00034
1.97968					

A33	1.81508	0.00001	0.00006	0.00001	0.00007
1.81515					
A34	1.89362	0.00002	-0.00007	0.00030	0.00022
1.89384					
A35	1.96293	0.00003	0.00014	0.00020	0.00034
1.96327					
A36	1.88749	-0.00003	-0.00008	-0.00025	-0.00033
1.88716					
A37	2.09564	0.00000	0.00000	0.00002	0.00002
2.09566					
A38	2.08625	0.00001	0.00001	0.00000	0.00001
2.08626					
A39	2.10128	-0.00001	-0.00002	-0.00001	-0.00003
2.10125					
A40	2.11684	-0.00001	0.00000	-0.00002	-0.00001
2.11682					
A41	2.08679	0.00001	0.00004	-0.00002	0.00002
2.08681					
A42	2.07946	0.00000	-0.00004	0.00003	-0.00001
2.07946					
A43	2.08471	0.00001	0.00001	0.00001	0.00003
2.08473					
A44	2.10356	-0.00001	-0.00001	-0.00001	-0.00002
2.10355					
A45	2.09486	0.00000	0.00000	-0.00001	-0.00001
2.09485					
A46	2.09572	0.00000	-0.00002	0.00001	-0.00001
2.09571					
A47	2.09192	0.00000	0.00000	0.00001	0.00001
2.09193					
A48	2.09549	0.00000	0.00001	-0.00001	0.00000
2.09549					
A49	2.09609	0.00000	0.00000	0.00001	0.00001
2.09610					
A50	2.08592	0.00002	0.00003	0.00000	0.00002
2.08594					
A51	2.10118	-0.00001	-0.00002	-0.00001	-0.00003
2.10115					
A52	2.09156	0.00000	0.00000	0.00000	0.00001
2.09157					
A53	2.09592	0.00000	-0.00001	0.00002	0.00001
2.09592					
A54	2.09570	0.00000	0.00001	-0.00002	-0.00001
2.09568					
A55	2.09517	0.00000	-0.00001	0.00001	0.00000
2.09517					
A56	2.10299	-0.00001	-0.00001	-0.00002	-0.00003
2.10296					
A57	2.08502	0.00001	0.00002	0.00001	0.00003
2.08505					
A58	2.08465	0.00001	0.00003	-0.00001	0.00003
2.08467					

This journal is © The Royal Society of Chemistry 2014

A59	2.11330	0.00001	0.00001	0.00008	0.00008
2.11339					
A60	2.08518	-0.00002	-0.00004	-0.00007	-0.00011
2.08507					
A61	1.91731	0.00001	-0.00004	0.00011	0.00008
1.91738					
A62	2.24242	-0.00001	0.00010	-0.00020	-0.00010
2.24233					
A63	2.12345	0.00000	-0.00006	0.00008	0.00002
2.12347					
A64	1.91462	-0.00003	-0.00001	-0.00010	-0.00011
1.91451					
A65	2.25419	0.00003	-0.00002	0.00019	0.00017
2.25436					
A66	2.11438	0.00000	0.00002	-0.00009	-0.00006
2.11432					
A67	1.94629	0.00002	0.00004	0.00004	0.00007
1.94636					
A68	2.02821	0.00000	0.00018	-0.00023	-0.00004
2.02817					
A69	2.15155	0.00006	-0.00004	0.00026	0.00022
2.15177					
A70	2.10088	-0.00005	-0.00013	-0.00005	-0.00018
2.10069					
D1	-3.13987	0.00000	-0.00006	0.00013	0.00006	-
3.13981					
D2	-1.04067	-0.00001	-0.00002	0.00013	0.00011	-
1.04056					
D3	0.96048	0.00001	-0.00002	0.00024	0.00021
0.96069					
D4	-0.02733	0.00000	0.00000	-0.00001	-0.00001	-
0.02733					
D5	2.07188	-0.00001	0.00004	-0.00001	0.00004
2.07191					
D6	-2.21016	0.00001	0.00004	0.00010	0.00015	-
2.21001					
D7	-0.02696	-0.00001	0.00000	-0.00017	-0.00017	-
0.02713					
D8	3.10526	0.00000	0.00013	-0.00016	-0.00003
3.10523					
D9	-3.14129	0.00000	-0.00006	-0.00004	-0.00010	-
3.14139					
D10	-0.00906	0.00000	0.00007	-0.00003	0.00004	-
0.00902					
D11	0.02580	0.00000	-0.00004	0.00005	0.00002
0.02581					
D12	-3.11816	0.00000	-0.00010	0.00014	0.00004	-
3.11812					
D13	3.13649	0.00000	0.00003	-0.00009	-0.00006
3.13643					
D14	-0.00747	0.00000	-0.00003	-0.00001	-0.00004	-
0.00750					

This journal is © The Royal Society of Chemistry 2014

D15	-1.09467	0.00001	-0.00025	0.00019	-0.00006	-1.09473
D16	1.07156	0.00001	-0.00020	0.00006	-0.00013	1.07143
D17	3.09722	0.00001	-0.00019	0.00005	-0.00014	3.09708
D18	1.03489	0.00000	-0.00022	0.00015	-0.00006	1.03482
D19	-3.08207	0.00001	-0.00016	0.00003	-0.00013	-3.08220
D20	-1.05641	0.00000	-0.00016	0.00002	-0.00015	-1.05655
D21	-3.09218	0.00000	-0.00026	0.00018	-0.00008	-3.09227
D22	-0.92595	0.00000	-0.00021	0.00005	-0.00015	-0.92611
D23	1.09971	0.00000	-0.00021	0.00004	-0.00017	1.09954
D24	-0.93642	0.00000	-0.00004	0.00000	-0.00004	-0.93645
D25	2.21693	0.00000	-0.00002	-0.00001	-0.00003	2.21690
D26	-3.12341	0.00000	-0.00003	0.00012	0.00009	-3.12331
D27	0.02994	0.00000	-0.00001	0.00011	0.00010	0.03004
D28	1.02754	0.00000	-0.00002	0.00007	0.00005	1.02759
D29	-2.10230	0.00000	0.00000	0.00005	0.00005	-2.10225
D30	-0.92304	0.00001	0.00007	0.00006	0.00013	-0.92291
D31	1.04268	0.00000	0.00006	0.00012	0.00018	1.04286
D32	-3.13208	0.00002	-0.00012	0.00057	0.00045	-3.13163
D33	2.22869	0.00000	-0.00007	0.00005	-0.00002	2.22867
D34	-2.08878	0.00000	-0.00008	0.00010	0.00003	-2.08875
D35	0.01965	0.00001	-0.00026	0.00056	0.00030	0.01995
D36	0.01883	0.00000	-0.00005	0.00009	0.00004	0.01887
D37	-3.11122	0.00000	-0.00008	0.00001	-0.00006	-3.11128
D38	-3.13352	0.00001	0.00010	0.00011	0.00021	-3.13331
D39	0.01962	0.00000	0.00007	0.00003	0.00010	0.01972
D40	-0.08363	-0.00001	0.00033	-0.00014	0.00019	-0.08344

This journal is © The Royal Society of Chemistry 2014

D41	-2.21192	-0.00002	0.00045	-0.00033	0.00012	-2.21179
D42	2.02478	0.00002	0.00053	0.00012	0.00065	2.02543
D43	2.03695	-0.00001	0.00034	-0.00029	0.00005	2.03700
D44	-0.09133	-0.00002	0.00046	-0.00048	-0.00002	-0.09135
D45	-2.13782	0.00002	0.00054	-0.00003	0.00051	-2.13731
D46	-2.19537	0.00000	0.00036	-0.00025	0.00011	-2.19526
D47	1.95953	-0.00001	0.00048	-0.00044	0.00005	1.95957
D48	-0.08696	0.00003	0.00056	0.00001	0.00057	-0.08639
D49	-2.02524	-0.00003	-0.00050	0.00011	-0.00039	-2.02563
D50	1.11181	0.00002	0.00037	0.00038	0.00075	1.11256
D51	2.16155	-0.00002	-0.00044	0.00006	-0.00038	2.16117
D52	-0.98459	0.00003	0.00044	0.00033	0.00077	-0.98382
D53	0.05270	-0.00003	-0.00048	0.00008	-0.00040	0.05229
D54	-3.09344	0.00002	0.00040	0.00035	0.00074	-3.09270
D55	-0.02328	0.00000	0.00011	-0.00018	-0.00007	-0.02335
D56	-3.11647	0.00000	-0.00004	0.00002	-0.00002	-3.11649
D57	3.10721	0.00000	0.00008	-0.00016	-0.00008	3.10714
D58	0.01402	0.00000	-0.00006	0.00004	-0.00002	0.01400
D59	-0.00139	0.00000	0.00003	0.00005	0.00008	-0.00131
D60	3.13477	0.00000	0.00003	0.00007	0.00009	3.13486
D61	-3.13052	0.00000	0.00005	0.00003	0.00009	-3.13043
D62	0.00564	0.00000	0.00005	0.00005	0.00010	0.00574
D63	0.94722	0.00000	-0.00012	0.00017	0.00005	0.94727
D64	-1.01314	0.00001	0.00004	0.00013	0.00017	-1.01296
D65	3.09483	-0.00001	0.00010	-0.00036	-0.00026	3.09457
D66	-2.24721	0.00000	0.00004	-0.00004	-0.00001	-2.24722

D67	2.07562	0.00001	0.00020	-0.00008	0.00011	2.07573
D68	-0.09960	-0.00001	0.00026	-0.00058	-0.00032	-0.09992
D69	3.10204	0.00000	0.00010	-0.00017	-0.00007	3.10197
D70	-0.02443	0.00000	0.00003	-0.00013	-0.00010	-0.02453
D71	0.01654	0.00000	-0.00007	0.00006	-0.00001	0.01653
D72	-3.10993	0.00000	-0.00014	0.00011	-0.00004	-3.10997
D73	-0.93665	0.00000	-0.00027	0.00008	-0.00020	-0.93684
D74	1.24192	0.00000	-0.00036	-0.00009	-0.00045	1.24146
D75	-2.95412	-0.00002	-0.00043	-0.00007	-0.00051	-2.95463
D76	1.04236	-0.00001	-0.00028	0.00000	-0.00028	1.04208
D77	-3.06225	-0.00001	-0.00037	-0.00017	-0.00054	-3.06280
D78	-0.97511	-0.00003	-0.00044	-0.00015	-0.00060	-0.97570
D79	-3.02367	0.00000	-0.00023	0.00007	-0.00017	-3.02384
D80	-0.84511	0.00000	-0.00032	-0.00010	-0.00043	-0.84554
D81	1.24204	-0.00002	-0.00040	-0.00009	-0.00048	1.24156
D82	1.61615	-0.00001	0.00127	-0.00396	-0.00269	1.61346
D83	-1.44887	-0.00002	0.00100	-0.00367	-0.00267	-1.45154
D84	-0.50466	0.00001	0.00108	-0.00346	-0.00238	-0.50704
D85	2.71351	-0.00001	0.00081	-0.00318	-0.00237	2.71114
D86	-2.62614	-0.00001	0.00105	-0.00375	-0.00270	-2.62885
D87	0.59203	-0.00002	0.00078	-0.00347	-0.00269	0.58934
D88	0.09731	-0.00003	-0.00048	-0.00011	-0.00059	0.09672
D89	-3.04575	0.00001	0.00044	-0.00015	0.00028	-3.04547
D90	2.18006	-0.00002	-0.00038	0.00004	-0.00034	2.17973
D91	-0.96300	0.00002	0.00054	-0.00001	0.00054	-0.96246
D92	-2.01242	-0.00001	-0.00044	0.00037	-0.00007	-2.01249

This journal is © The Royal Society of Chemistry 2014

D93	1.12770	0.00003	0.00048	0.00032	0.00080	1.12850
D94	-0.01471	0.00000	-0.00001	-0.00005	-0.00006	-0.01477
D95	3.13779	0.00000	0.00004	-0.00001	0.00003	3.13782
D96	3.12143	0.00000	-0.00001	-0.00004	-0.00004	3.12139
D97	-0.00925	0.00000	0.00005	0.00000	0.00005	-0.00920
D98	-3.13750	0.00000	-0.00002	0.00000	-0.00001	-3.13751
D99	0.01550	0.00000	0.00002	0.00012	0.00014	0.01564
D100	0.01889	0.00000	-0.00009	0.00005	-0.00004	0.01885
D101	-3.11130	0.00000	-0.00005	0.00017	0.00012	-3.11118
D102	0.00419	0.00000	-0.00003	-0.00003	-0.00006	0.00413
D103	3.13485	-0.00001	-0.00008	-0.00007	-0.00015	3.13470
D104	-3.12593	0.00000	0.00001	0.00009	0.00009	-3.12584
D105	0.00472	0.00000	-0.00005	0.00005	0.00001	0.00473
D106	-3.13274	0.00000	-0.00001	0.00001	-0.00001	-3.13274
D107	0.01408	0.00000	-0.00003	-0.00001	-0.00005	0.01403
D108	0.00648	0.00000	-0.00007	0.00009	0.00002	0.00650
D109	-3.12989	0.00000	-0.00009	0.00007	-0.00003	-3.12992
D110	3.13260	0.00000	0.00002	0.00000	0.00002	3.13262
D111	-0.00424	0.00000	0.00006	0.00007	0.00013	-0.00411
D112	-0.00376	0.00000	0.00000	-0.00002	-0.00002	-0.00378
D113	-3.14060	0.00000	0.00003	0.00005	0.00009	-3.14051
D114	-0.01227	0.00000	-0.00001	-0.00011	-0.00013	-0.01239
D115	3.11797	0.00000	0.00002	-0.00004	-0.00002	3.11795
D116	3.13405	0.00000	0.00002	-0.00004	-0.00002	3.13403
D117	-0.01890	0.00000	0.00005	0.00004	0.00009	-0.01881
D118	0.00886	0.00001	0.00018	-0.00015	0.00004	0.00889

```
   D119      -3.12856  -0.00003  -0.00062  -0.00040  -0.00102  -
3.12958
   D120      -0.06888   0.00001   0.00020   0.00016   0.00036  -
0.06852
   D121       3.07404  -0.00002  -0.00063   0.00020  -0.00043
3.07361
         Item               Value     Threshold  Converged?
 Maximum Force            0.000124     0.000450     YES
 RMS     Force            0.000026     0.000300     YES
 Maximum Displacement     0.004749     0.001800     NO
 RMS     Displacement     0.000551     0.001200     YES
 Predicted change in Energy=-3.563453D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.620102   -1.033987   -0.392888
      2          6           0       -0.184772   -1.436150   -0.666726
      3          1           0       -0.093757   -2.444860   -1.076886
      4          6           0       -1.748863    0.263588    0.133167
      5          6           0        0.337815   -0.373897   -1.701336
      6          1           0       -0.251949   -0.458862   -2.618881
      7          6           0        0.596528   -1.256319    0.622229
      8          6           0        0.479350    0.028408    1.187469
      9          6           0       -0.391932    0.970936    0.348199
     10          6           0        0.281452    1.033308   -1.074226
     11          1           0       -0.262910    1.760144   -1.684674
     12          6           0        1.386258   -2.228446    1.232378
     13          1           0        1.479825   -3.214751    0.784069
     14          6           0        1.172834    0.335770    2.359011
     15          1           0        1.129379    1.328707    2.795868
     16          6           0        1.955785   -0.647771    2.977004
     17          1           0        2.491828   -0.407490    3.891121
     18          6           0        2.061279   -1.923478    2.420157
     19          1           0        2.675821   -2.678767    2.902373
     20          6           0       -2.749218   -1.808302   -0.646450
     21          1           0       -2.642827   -2.809601   -1.057977
     22          6           0       -4.019446   -1.289136   -0.365113
     23          1           0       -4.903790   -1.892037   -0.553239
     24          6           0       -4.149472    0.001605    0.149742
     25          1           0       -5.135608    0.406718    0.359883
     26          6           0       -3.014844    0.787312    0.394495
     27          1           0       -3.136336    1.797322    0.774434
     28          6           0        1.801108   -0.576869   -2.057702
     29          6           0        1.743823    1.467743   -1.009523
     30          8           0        2.544267    0.516912   -1.638582
     31          8           0        2.219517    2.450430   -0.518762
```

32	8	0	2.311738	-1.510183	-2.610901
33	6	0	-0.616080	2.360455	0.931249
34	1	0	-0.595190	2.436510	2.036029
35	8	0	-0.884523	3.329475	0.255803

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515551	0.000000			
3	H	2.188183	1.092708	0.000000		
4	C	1.406064	2.444446	3.396953	0.000000	
5	C	2.445648	1.572227	2.205692	2.850616	0.000000
6	H	2.675379	2.184151	2.519317	3.215035	1.094043
7	C	2.448130	1.517950	2.185432	2.837280	2.498911
8	C	2.834415	2.454389	3.401883	2.476246	2.920115
9	C	2.465224	2.620506	3.713144	1.545264	2.557675
10	C	2.890301	2.545908	3.498349	2.484441	1.541646
11	H	3.364201	3.355387	4.252067	2.784292	2.217043
12	C	3.620279	2.588911	2.751360	4.153009	3.625639
13	H	3.968691	2.835332	2.555787	4.790296	3.943587
14	C	4.153273	3.760037	4.597994	3.673677	4.205627
15	H	4.828057	4.621795	5.543834	4.063094	4.873426
16	C	4.928722	4.298871	4.885097	4.758403	4.957792
17	H	5.971030	5.384821	5.959633	5.705789	5.993035
18	C	4.717730	3.848516	4.140692	4.952854	4.728449
19	H	5.658533	4.739784	4.853841	5.991976	5.654452
20	C	1.392394	2.591388	2.764408	2.429247	3.563716
21	H	2.154324	2.842794	2.575102	3.415038	3.902664
22	C	2.413032	3.849326	4.153715	2.795493	4.648535
23	H	3.397730	4.742346	4.869932	3.882195	5.576495
24	C	2.786506	4.295650	4.892712	2.414919	4.868597
25	H	3.873122	5.381530	5.967919	3.397342	5.900537
26	C	2.425368	3.752237	4.598331	1.394736	4.120829
27	H	3.417297	4.609123	5.539023	2.165328	4.786789
28	C	3.832132	2.572333	2.835825	4.255416	1.519678
29	C	4.237320	3.502797	4.323158	3.867116	2.418078
30	O	4.615085	3.493796	4.005842	4.651261	2.380317
31	O	5.186491	4.572528	5.443033	4.577699	3.593899
32	O	4.539351	3.165101	3.002204	5.211972	2.452515
33	C	3.779370	4.141710	5.234165	2.513361	3.913707
34	H	4.358261	4.740341	5.811149	3.110215	4.768311
35	O	4.472324	4.904273	5.978655	3.187756	4.363424

		6	7	8	9	10
6	H	0.000000				
7	C	3.443929	0.000000			
8	C	3.906472	1.408457	0.000000		
9	C	3.296587	2.452104	1.533579	0.000000	
10	C	2.212928	2.866989	2.482790	1.575001	0.000000
11	H	2.407665	3.893519	3.434976	2.184507	1.094197
12	C	4.543935	1.393192	2.432671	3.765604	4.144883
13	H	4.708931	2.154497	3.417859	4.605804	4.789088
14	C	5.238402	2.425549	1.395673	2.625889	3.615001

This journal is © The Royal Society of Chemistry 2014

15	H	5.867110	3.419211	2.168009	2.904044	3.972892
16	C	6.018613	2.786194	2.416509	3.878479	4.694878
17	H	7.064777	3.872767	3.398501	4.771627	5.622840
18	C	5.734808	2.413118	2.798550	4.323064	4.911322
19	H	6.632047	3.397921	3.885122	5.408811	5.943554
20	C	3.456562	3.620531	4.142513	3.777604	4.176446
21	H	3.698471	3.966005	4.779572	4.619126	4.829040
22	C	4.467981	4.720502	4.938177	4.333082	4.939060
23	H	5.287768	5.660332	5.974644	5.419047	5.976271
24	C	4.802915	4.932559	4.743795	3.885627	4.711221
25	H	5.785533	5.974270	5.688213	4.777127	5.638601
26	C	4.273988	4.155755	3.662531	2.629739	3.617074
27	H	4.992459	4.825160	4.046336	2.897644	3.960118
28	C	2.131640	3.015742	3.555916	3.604648	2.422653
29	C	3.207015	3.376302	2.915021	2.579084	1.526908
30	O	3.119606	3.471211	3.533989	3.574171	2.388618
31	O	4.356906	4.204277	3.435927	3.124130	2.464320
32	O	2.770890	3.668722	4.489156	4.714028	3.598998
33	C	4.548029	3.827136	2.589219	1.523467	2.566868
34	H	5.492648	4.129893	2.770135	2.244547	3.522948
35	O	4.797443	4.832938	3.691232	2.411201	2.898423

		11	12	13	14	15
11	H	0.000000				
12	C	5.209395	0.000000			
13	H	5.820773	1.087443	0.000000		
14	C	4.521238	2.808925	3.896265	0.000000	
15	H	4.711674	3.894076	4.981281	1.085659	0.000000
16	C	5.696658	2.422110	3.409528	1.400815	2.149936
17	H	6.586100	3.406917	4.307973	2.153960	2.463783
18	C	5.985029	1.399814	2.163852	2.428431	3.403866
19	H	7.027166	2.157462	2.490962	3.411985	4.296821
20	C	4.471403	4.561653	4.680736	5.386310	6.060849
21	H	5.190310	4.670867	4.533602	6.010694	6.797592
22	C	5.015069	5.714536	5.938905	6.084484	6.584474
23	H	6.013014	6.547236	6.654961	7.097161	7.615041
24	C	4.643588	6.065438	6.514316	5.772303	6.052227
25	H	5.454829	7.088023	7.553736	6.618005	6.784847
26	C	3.583642	5.400606	6.030782	4.647565	4.820195
27	H	3.782218	6.072098	6.813949	4.818295	4.743640
28	C	3.140214	3.704651	3.890670	4.553569	5.257337
29	C	2.137360	4.337716	5.021196	3.599223	3.857185
30	O	3.070503	4.137679	4.574668	4.230176	4.724963
31	O	2.828125	5.064849	5.859931	3.721412	3.665165
32	O	4.264006	4.017861	3.888889	5.422608	6.220163
33	C	2.707057	5.015780	5.957969	3.055825	2.754620
34	H	3.796251	5.131648	6.148971	2.764658	2.186028
35	O	2.571897	6.082815	6.978259	4.197436	3.809305

		16	17	18	19	20
16	C	0.000000				
17	H	1.086594	0.000000			
18	C	1.395935	2.155766	0.000000		
19	H	2.156145	2.483983	1.086579	0.000000	

20	C	6.050893	7.072509	5.705981	6.540863	0.000000
21	H	6.488591	7.525184	5.917030	6.632458	1.087783
22	C	6.876371	7.828762	6.718283	7.578531	1.400772
23	H	7.814383	8.755078	7.573259	8.367240	2.158212
24	C	6.759384	7.633619	6.887246	7.832368	2.422891
25	H	7.632112	8.444546	7.840263	8.775129	3.407914
26	C	5.782384	6.631544	6.100714	7.119467	2.809153
27	H	6.062960	6.800821	6.600602	7.638367	3.894778
28	C	5.037581	5.991184	4.683191	5.457604	4.920724
29	C	4.518044	5.300219	4.833618	5.776252	5.572406
30	O	4.796503	5.606683	4.760478	5.554273	5.866168
31	O	4.678545	5.262027	5.271941	6.182316	6.545337
32	O	5.665258	6.597322	5.054215	5.647507	5.437023
33	C	4.455225	5.107000	5.266610	6.333695	4.941452
34	H	4.111654	4.589050	5.119949	6.133198	5.463878
35	O	5.593816	6.211296	6.399664	7.468557	5.539666

		21	22	23	24	25
21	H	0.000000				
22	C	2.164938	0.000000			
23	H	2.491714	1.086713	0.000000		
24	C	3.410491	1.395706	2.156168	0.000000	
25	H	4.309175	2.155773	2.484312	1.086618	0.000000
26	C	3.896904	2.428553	3.412511	1.401650	2.154923
27	H	4.982471	3.406563	4.300928	2.154364	2.470369
28	C	5.072780	6.103362	6.996337	6.373135	7.411490
29	C	6.127048	6.421130	7.462377	6.182587	7.094196
30	O	6.189405	6.925739	7.902819	6.947646	7.936402
31	O	7.183389	7.275481	8.342645	6.856214	7.684182
32	O	5.352361	6.721333	7.512898	7.187065	8.243969
33	C	5.898661	5.155868	6.218670	4.319698	4.956782
34	H	6.425525	5.601022	6.633602	4.703165	5.248326
35	O	6.519655	5.616480	6.638768	4.663246	5.159948

		26	27	28	29	30
26	C	0.000000				
27	H	1.085925	0.000000			
28	C	5.573836	6.167343	0.000000		
29	C	5.007910	5.206446	2.298347	0.000000	
30	O	5.925389	6.303280	1.387193	1.393020	0.000000
31	O	5.567633	5.548339	3.421687	1.196999	2.257865
32	O	6.533251	7.216758	1.199103	3.428554	2.260219
33	C	2.918382	2.587161	4.837819	3.183186	4.471071
34	H	3.356965	2.908196	5.619727	3.960414	5.200367
35	O	3.319652	2.772568	5.274888	3.460535	4.822427

		31	32	33	34	35
31	O	0.000000				
32	O	4.480180	0.000000			
33	C	3.186101	6.008393	0.000000		
34	H	3.801280	6.754301	1.107592	0.000000	
35	O	3.317791	6.469650	1.211317	2.012537	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99

This journal is © The Royal Society of Chemistry 2014

```
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.622178   -1.025266   -0.411835
      2          6           0       -0.186179   -1.431061   -0.676662
      3          1           0       -0.095698   -2.436813   -1.094137
      4          6           0       -1.750239    0.268566    0.123529
      5          6           0        0.349482   -0.362687   -1.698202
      6          1           0       -0.232749   -0.437897   -2.621392
      7          6           0        0.584783   -1.264745    0.620307
      8          6           0        0.467918    0.015879    1.194847
      9          6           0       -0.392376    0.968640    0.355798
     10          6           0        0.293391    1.039666   -1.060291
     11          1           0       -0.242818    1.773579   -1.669486
     12          6           0        1.365370   -2.244936    1.229318
     13          1           0        1.458820   -3.227989    0.773901
     14          6           0        1.152583    0.311019    2.374690
     15          1           0        1.109367    1.300592    2.819138
     16          6           0        1.926279   -0.680622    2.991396
     17          1           0        2.455442   -0.449857    3.911951
     18          6           0        2.031424   -1.952245    2.425221
     19          1           0        2.638793   -2.713868    2.906561
     20          6           0       -2.752173   -1.792922   -0.681229
     21          1           0       -2.646275   -2.791316   -1.099880
     22          6           0       -4.022673   -1.270861   -0.406555
     23          1           0       -4.907782   -1.868631   -0.607054
     24          6           0       -4.151931    0.016232    0.117544
     25          1           0       -5.138199    0.423658    0.322529
     26          6           0       -3.016302    0.795328    0.378269
     27          1           0       -3.136996    1.802747    0.765274
     28          6           0        1.814945   -0.568751   -2.043711
     29          6           0        1.756882    1.467612   -0.979639
     30          8           0        2.558864    0.518603   -1.609488
     31          8           0        2.232291    2.444392   -0.476951
     32          8           0        2.326549   -1.499674   -2.600033
     33          6           0       -0.615940    2.354343    0.948080
     34          1           0       -0.604194    2.421458    2.053574
     35          8           0       -0.874717    3.329829    0.278191
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3746448      0.2672251
0.2547399
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   461 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
```

```
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1927.9745910538 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
                (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1032.18960873     A.U. after   12 cycles
            Convg  =    0.5464D-08             -V/T =  2.0093
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000033888   -0.000027352   -0.000010023
      2        6          -0.000009991   -0.000001583    0.000000403
      3        1          -0.000000012   -0.000004790    0.000001460
      4        6           0.000016113    0.000015855    0.000007918
      5        6          -0.000043681    0.000028778   -0.000001637
      6        1          -0.000001097    0.000000444    0.000001060
      7        6          -0.000019884   -0.000016108   -0.000021148
      8        6          -0.000004062    0.000015614   -0.000008353
      9        6           0.000031660   -0.000011651    0.000026089
     10        6          -0.000019923   -0.000032268   -0.000025418
     11        1           0.000005017    0.000001989   -0.000004816
     12        6           0.000003302   -0.000012924   -0.000009989
     13        1           0.000001140   -0.000007064   -0.000005573
     14        6           0.000009666    0.000019830    0.000009697
     15        1          -0.000004892    0.000001817   -0.000003486
     16        6           0.000012005    0.000003695    0.000019052
     17        1           0.000006954   -0.000004870    0.000001661
     18        6           0.000007628   -0.000014868    0.000004633
     19        1           0.000006847   -0.000006673   -0.000004121
     20        6           0.000000996   -0.000004885   -0.000008136
     21        1          -0.000003215   -0.000006599    0.000000040
     22        6          -0.000015094   -0.000009232    0.000000726
     23        1          -0.000006045   -0.000001228    0.000001361
     24        6          -0.000026620    0.000015595    0.000011820
     25        1          -0.000004982    0.000000399    0.000003512
     26        6          -0.000013287    0.000016387    0.000005523
     27        1          -0.000000270    0.000002975    0.000009132
     28        6           0.000039104    0.000020803    0.000007046
     29        6           0.000003455    0.000046150    0.000007614
     30        8          -0.000002604   -0.000031916   -0.000025659
     31        8           0.000018032   -0.000001592    0.000000335
     32        8           0.000002823   -0.000019430   -0.000010880
     33        6          -0.000045758    0.000052949   -0.000042136
     34        1           0.000000695   -0.000008893    0.000015548
     35        8           0.000022090   -0.000019356    0.000046743
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000052949 RMS     0.000017396
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000044528 RMS     0.000010857
 Search for a local minimum.
 Step number   8 out of a maximum of  210
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8
 DE= -7.60D-07 DEPred=-3.56D-07 R= 2.13D+00
 Trust test= 2.13D+00 RLast= 7.08D-03 DXMaxT set to 6.21D-02
     Eigenvalues ---    0.00195   0.00489   0.01099   0.01124
0.01164
     Eigenvalues ---    0.01427   0.01486   0.01621   0.01801
0.02049
     Eigenvalues ---    0.02116   0.02121   0.02130   0.02132
0.02135
     Eigenvalues ---    0.02139   0.02145   0.02147   0.02157
0.02160
     Eigenvalues ---    0.02163   0.02173   0.02806   0.03853
0.03927
     Eigenvalues ---    0.04651   0.04892   0.04946   0.05251
0.05323
     Eigenvalues ---    0.05496   0.05606   0.06211   0.06592
0.08345
     Eigenvalues ---    0.09036   0.09398   0.10001   0.12422
0.15714
     Eigenvalues ---    0.15945   0.15999   0.16000   0.16000
0.16001
     Eigenvalues ---    0.16002   0.16004   0.16046   0.16634
0.20320
     Eigenvalues ---    0.20756   0.21985   0.22000   0.22010
0.22614
     Eigenvalues ---    0.22710   0.22831   0.23938   0.24531
0.24638
     Eigenvalues ---    0.24707   0.25031   0.26621   0.27335
0.28387
     Eigenvalues ---    0.28768   0.28848   0.29772   0.30437
0.30899
     Eigenvalues ---    0.32618   0.34392   0.34413   0.34530
0.35129
     Eigenvalues ---    0.35170   0.35234   0.35244   0.35248
0.35308
     Eigenvalues ---    0.35349   0.35439   0.36708   0.40042
0.41964
```

```
     Eigenvalues ---    0.42099   0.42498   0.43578   0.44191
0.44834
     Eigenvalues ---    0.46052   0.46198   0.46326   0.46455
0.46817
     Eigenvalues ---    0.49102   0.99514   1.04757
1.059371000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     8    7    6    5
4
 RFO step:  Lambda=-5.46399416D-08.
 DIIS coeffs:      1.65220     -0.42813     -0.19897     -0.02832
0.00322
 Iteration  1 RMS(Cart)=  0.00076251 RMS(Int)=  0.00000126
 Iteration  2 RMS(Cart)=  0.00000133 RMS(Int)=  0.00000018
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000018
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86398  -0.00001   0.00006  -0.00007  -0.00001
2.86396
    R2        2.65708   0.00003   0.00000   0.00004   0.00004
2.65712
    R3        2.63124   0.00002   0.00002   0.00001   0.00003
2.63128
    R4        2.06492   0.00000   0.00000   0.00001   0.00001
2.06493
    R5        2.97108   0.00001  -0.00003   0.00002  -0.00001
2.97107
    R6        2.86851   0.00001   0.00000   0.00003   0.00003
2.86854
    R7        2.92013   0.00002   0.00008   0.00005   0.00014
2.92026
    R8        2.63567   0.00004   0.00004   0.00004   0.00008
2.63575
    R9        2.06744   0.00000   0.00000  -0.00001  -0.00001
2.06743
   R10        2.91329   0.00000   0.00016  -0.00001   0.00015
2.91344
   R11        2.87177   0.00003  -0.00005   0.00011   0.00006
2.87183
   R12        2.66160   0.00003  -0.00001   0.00003   0.00003
2.66162
   R13        2.63275   0.00002   0.00003   0.00001   0.00004
2.63279
   R14        2.89804   0.00000   0.00016  -0.00011   0.00006
2.89810
   R15        2.63744   0.00002   0.00001   0.00001   0.00002
2.63746
   R16        2.97632   0.00004  -0.00020   0.00008  -0.00012
2.97620
   R17        2.87894   0.00003  -0.00008   0.00005  -0.00003
2.87890
```

R18	2.06773	0.00000	0.00003	-0.00001	0.00002
2.06775					
R19	2.88544	0.00004	0.00000	0.00015	0.00015
2.88559					
R20	2.05497	0.00001	0.00001	0.00001	0.00001
2.05498					
R21	2.64526	0.00003	0.00003	0.00003	0.00006
2.64532					
R22	2.05160	0.00000	0.00000	0.00001	0.00002
2.05162					
R23	2.64716	0.00002	0.00004	0.00001	0.00005
2.64721					
R24	2.05337	0.00001	0.00001	0.00000	0.00001
2.05338					
R25	2.63794	0.00003	0.00002	0.00003	0.00005
2.63799					
R26	2.05334	0.00001	0.00001	0.00001	0.00001
2.05335					
R27	2.05561	0.00001	0.00001	0.00001	0.00002
2.05563					
R28	2.64708	0.00003	0.00004	0.00002	0.00006
2.64713					
R29	2.05359	0.00001	0.00001	0.00001	0.00001
2.05361					
R30	2.63750	0.00002	0.00001	0.00002	0.00003
2.63754					
R31	2.05341	0.00000	0.00001	0.00000	0.00001
2.05342					
R32	2.64873	0.00003	0.00004	0.00002	0.00006
2.64880					
R33	2.05210	0.00000	0.00001	0.00002	0.00003
2.05213					
R34	2.62141	-0.00002	-0.00018	-0.00008	-0.00026
2.62115					
R35	2.26598	0.00002	0.00008	0.00000	0.00008
2.26606					
R36	2.63243	0.00003	0.00022	0.00008	0.00030
2.63273					
R37	2.26200	0.00001	-0.00004	-0.00002	-0.00006
2.26194					
R38	2.09305	0.00001	0.00001	0.00007	0.00008
2.09312					
R39	2.28906	-0.00004	0.00003	-0.00007	-0.00004
2.28901					
A1	1.98145	0.00000	0.00000	-0.00003	-0.00004
1.98142					
A2	2.19879	0.00000	0.00000	0.00005	0.00005
2.19884					
A3	2.10258	-0.00001	0.00000	-0.00002	-0.00001
2.10256					
A4	1.97324	0.00000	-0.00004	0.00002	-0.00001
1.97322					

This journal is © The Royal Society of Chemistry 2014

A5	1.82803	0.00000	0.00002	-0.00009	-0.00007
1.82796					
A6	1.87821	0.00000	-0.00003	0.00004	0.00000
1.87822					
A7	1.92731	0.00000	0.00001	0.00003	0.00004
1.92735					
A8	1.96625	0.00000	-0.00002	-0.00001	-0.00003
1.96622					
A9	1.88353	0.00000	0.00008	-0.00001	0.00007
1.88360					
A10	1.97586	-0.00001	-0.00001	0.00004	0.00003
1.97589					
A11	2.09411	0.00000	0.00000	-0.00001	0.00000
2.09410					
A12	2.21317	0.00001	0.00001	-0.00003	-0.00002
2.21315					
A13	1.89678	0.00000	-0.00005	0.00001	-0.00004
1.89675					
A14	1.91440	0.00001	-0.00004	0.00008	0.00003
1.91443					
A15	1.96506	-0.00001	0.00011	-0.00014	-0.00003
1.96503					
A16	1.97397	0.00000	-0.00002	0.00000	-0.00001
1.97395					
A17	1.88812	0.00000	0.00003	0.00000	0.00003
1.88815					
A18	1.82607	0.00000	-0.00003	0.00004	0.00002
1.82609					
A19	1.98889	0.00000	-0.00003	0.00003	0.00000
1.98889					
A20	2.19073	0.00001	0.00004	0.00003	0.00007
2.19080					
A21	2.10351	-0.00001	-0.00001	-0.00006	-0.00007
2.10344					
A22	1.96952	0.00000	0.00001	-0.00001	0.00000
1.96953					
A23	2.09026	0.00001	0.00002	0.00008	0.00010
2.09036					
A24	2.22223	-0.00001	-0.00004	-0.00007	-0.00011
2.22212					
A25	1.86891	0.00000	-0.00009	0.00004	-0.00004
1.86886					
A26	1.84200	-0.00001	0.00004	0.00004	0.00008
1.84208					
A27	1.91938	-0.00001	-0.00016	-0.00018	-0.00034
1.91904					
A28	1.85010	0.00000	0.00005	-0.00008	-0.00003
1.85006					
A29	2.02050	-0.00001	-0.00015	-0.00011	-0.00026
2.02024					
A30	1.95241	0.00002	0.00032	0.00029	0.00061
1.95303					

This journal is © The Royal Society of Chemistry 2014

A31	1.92501	0.00000	0.00002	-0.00008	-0.00006
1.92495					
A32	1.97968	0.00000	-0.00022	0.00005	-0.00016
1.97952					
A33	1.81515	0.00000	0.00000	-0.00005	-0.00005
1.81510					
A34	1.89384	0.00000	0.00020	0.00001	0.00021
1.89405					
A35	1.96327	0.00001	0.00016	0.00009	0.00025
1.96352					
A36	1.88716	0.00000	-0.00018	-0.00003	-0.00020
1.88696					
A37	2.09566	0.00000	0.00001	0.00000	0.00001
2.09567					
A38	2.08626	0.00000	0.00000	0.00000	0.00000
2.08627					
A39	2.10125	0.00000	-0.00001	0.00000	-0.00001
2.10123					
A40	2.11682	-0.00001	-0.00001	-0.00006	-0.00007
2.11675					
A41	2.08681	0.00000	-0.00001	-0.00003	-0.00004
2.08677					
A42	2.07946	0.00001	0.00002	0.00009	0.00011
2.07957					
A43	2.08473	0.00001	0.00001	0.00003	0.00004
2.08477					
A44	2.10355	-0.00001	-0.00001	-0.00003	-0.00003
2.10351					
A45	2.09485	0.00000	0.00000	0.00000	0.00000
2.09485					
A46	2.09571	0.00000	0.00000	0.00004	0.00004
2.09575					
A47	2.09193	0.00000	0.00000	-0.00003	-0.00002
2.09191					
A48	2.09549	0.00000	-0.00001	-0.00001	-0.00002
2.09547					
A49	2.09610	0.00000	0.00001	0.00000	0.00001
2.09611					
A50	2.08594	0.00001	0.00000	0.00001	0.00001
2.08596					
A51	2.10115	-0.00001	-0.00001	-0.00002	-0.00003
2.10112					
A52	2.09157	0.00000	0.00000	-0.00001	-0.00001
2.09155					
A53	2.09592	0.00000	0.00001	0.00001	0.00002
2.09594					
A54	2.09568	0.00000	-0.00001	0.00000	-0.00001
2.09568					
A55	2.09517	0.00000	0.00000	-0.00001	0.00000
2.09516					
A56	2.10296	-0.00001	-0.00001	-0.00002	-0.00003
2.10293					

A57	2.08505	0.00001	0.00001	0.00003	0.00004	2.08508
A58	2.08467	0.00001	0.00000	0.00002	0.00002	2.08469
A59	2.11339	0.00000	0.00005	-0.00003	0.00003	2.11341
A60	2.08507	0.00000	-0.00005	0.00001	-0.00005	2.08502
A61	1.91738	0.00000	0.00007	-0.00002	0.00006	1.91744
A62	2.24233	-0.00001	-0.00012	-0.00003	-0.00015	2.24218
A63	2.12347	0.00000	0.00005	0.00004	0.00009	2.12356
A64	1.91451	-0.00001	-0.00007	-0.00002	-0.00009	1.91442
A65	2.25436	0.00002	0.00013	0.00011	0.00024	2.25460
A66	2.11432	-0.00001	-0.00007	-0.00008	-0.00015	2.11416
A67	1.94636	0.00001	0.00003	0.00003	0.00006	1.94642
A68	2.02817	-0.00003	-0.00013	-0.00028	-0.00041	2.02776
A69	2.15177	0.00004	0.00018	0.00022	0.00040	2.15217
A70	2.10069	-0.00001	-0.00005	0.00006	0.00001	2.10070
D1	-3.13981	0.00000	0.00008	-0.00008	0.00000	-3.13980
D2	-1.04056	0.00000	0.00008	-0.00008	0.00000	-1.04056
D3	0.96069	0.00000	0.00016	-0.00011	0.00005	0.96075
D4	-0.02733	0.00000	0.00000	-0.00012	-0.00012	-0.02745
D5	2.07191	0.00000	0.00000	-0.00012	-0.00012	2.07180
D6	-2.21001	0.00000	0.00008	-0.00015	-0.00007	-2.21008
D7	-0.02713	0.00000	-0.00011	0.00009	-0.00003	-0.02716
D8	3.10523	0.00000	-0.00008	-0.00005	-0.00013	3.10510
D9	-3.14139	0.00000	-0.00004	0.00012	0.00008	-3.14131
D10	-0.00902	0.00000	-0.00001	-0.00001	-0.00002	-0.00905
D11	0.02581	0.00000	0.00003	0.00011	0.00014	0.02595
D12	-3.11812	0.00000	0.00007	0.00004	0.00012	-3.11800

This journal is © The Royal Society of Chemistry 2014

D13	3.13643	0.00000	-0.00006	0.00007	0.00001	3.13645
D14	-0.00750	0.00000	-0.00001	0.00000	-0.00001	-0.00751
D15	-1.09473	0.00000	0.00014	0.00014	0.00029	-1.09445
D16	1.07143	0.00001	0.00006	0.00020	0.00027	1.07169
D17	3.09708	0.00001	0.00007	0.00022	0.00029	3.09736
D18	1.03482	0.00000	0.00011	0.00014	0.00025	1.03507
D19	-3.08220	0.00000	0.00003	0.00020	0.00023	-3.08197
D20	-1.05655	0.00001	0.00004	0.00022	0.00025	-1.05630
D21	-3.09227	0.00000	0.00014	0.00014	0.00028	-3.09199
D22	-0.92611	0.00000	0.00006	0.00021	0.00026	-0.92584
D23	1.09954	0.00001	0.00006	0.00022	0.00029	1.09983
D24	-0.93645	0.00000	0.00000	-0.00007	-0.00006	-0.93651
D25	2.21690	0.00000	-0.00002	0.00009	0.00007	2.21697
D26	-3.12331	0.00000	0.00009	-0.00012	-0.00003	-3.12334
D27	0.03004	0.00000	0.00007	0.00004	0.00011	0.03014
D28	1.02759	0.00000	0.00004	-0.00015	-0.00011	1.02748
D29	-2.10225	0.00000	0.00002	0.00001	0.00002	-2.10223
D30	-0.92291	0.00000	0.00004	-0.00002	0.00002	-0.92289
D31	1.04286	0.00000	0.00007	-0.00007	0.00000	1.04286
D32	-3.13163	0.00001	0.00039	0.00020	0.00059	-3.13104
D33	2.22867	0.00000	0.00001	0.00013	0.00014	2.22880
D34	-2.08875	-0.00001	0.00004	0.00007	0.00011	-2.08864
D35	0.01995	0.00001	0.00036	0.00035	0.00071	0.02066
D36	0.01887	0.00000	0.00005	-0.00003	0.00002	0.01889
D37	-3.11128	0.00000	0.00000	-0.00003	-0.00004	-3.11132
D38	-3.13331	0.00000	0.00008	-0.00018	-0.00010	-3.13341

This journal is © The Royal Society of Chemistry 2014

D39	0.01972	0.00000	0.00003	-0.00019	-0.00016	0.01956
D40	-0.08344	0.00000	-0.00011	-0.00021	-0.00032	-0.08376
D41	-2.21179	0.00000	-0.00023	-0.00021	-0.00044	-2.21224
D42	2.02543	0.00000	0.00009	-0.00017	-0.00009	2.02534
D43	2.03700	0.00000	-0.00022	-0.00014	-0.00036	2.03665
D44	-0.09135	0.00000	-0.00034	-0.00014	-0.00048	-0.09183
D45	-2.13731	0.00000	-0.00002	-0.00010	-0.00012	-2.13743
D46	-2.19526	0.00000	-0.00020	-0.00011	-0.00031	-2.19557
D47	1.95957	0.00000	-0.00032	-0.00011	-0.00043	1.95914
D48	-0.08639	0.00001	0.00000	-0.00007	-0.00007	-0.08646
D49	-2.02563	-0.00001	0.00012	-0.00015	-0.00003	-2.02567
D50	1.11256	-0.00001	0.00018	-0.00015	0.00004	1.11260
D51	2.16117	0.00000	0.00009	-0.00008	0.00001	2.16118
D52	-0.98382	0.00000	0.00015	-0.00007	0.00008	-0.98374
D53	0.05229	0.00000	0.00011	-0.00011	0.00000	0.05229
D54	-3.09270	0.00000	0.00017	-0.00010	0.00007	-3.09263
D55	-0.02335	0.00000	-0.00012	0.00012	0.00000	-0.02335
D56	-3.11649	0.00000	-0.00001	0.00008	0.00007	-3.11642
D57	3.10714	0.00000	-0.00010	-0.00002	-0.00012	3.10701
D58	0.01400	0.00000	0.00002	-0.00007	-0.00005	0.01394
D59	-0.00131	0.00000	0.00005	-0.00009	-0.00004	-0.00135
D60	3.13486	0.00000	0.00006	-0.00010	-0.00005	3.13482
D61	-3.13043	0.00000	0.00003	0.00008	0.00010	-3.13033
D62	0.00574	0.00000	0.00003	0.00006	0.00009	0.00584
D63	0.94727	0.00000	0.00012	-0.00014	-0.00002	0.94725
D64	-1.01296	0.00000	0.00009	-0.00017	-0.00008	-1.01304

This journal is © The Royal Society of Chemistry 2014

D65	3.09457	-0.00002	-0.00026	-0.00042	-0.00067	3.09389
D66	-2.24722	0.00000	0.00000	-0.00009	-0.00009	-2.24731
D67	2.07573	0.00001	-0.00003	-0.00012	-0.00015	2.07558
D68	-0.09992	-0.00001	-0.00038	-0.00037	-0.00075	-0.10067
D69	3.10197	0.00000	-0.00011	0.00015	0.00004	3.10201
D70	-0.02453	0.00000	-0.00007	0.00003	-0.00004	-0.02457
D71	0.01653	0.00000	0.00003	0.00009	0.00012	0.01665
D72	-3.10997	0.00000	0.00006	-0.00002	0.00004	-3.10993
D73	-0.93684	0.00000	0.00007	0.00019	0.00026	-0.93658
D74	1.24146	0.00000	-0.00005	0.00022	0.00016	1.24163
D75	-2.95463	0.00000	-0.00004	0.00025	0.00021	-2.95442
D76	1.04208	0.00000	0.00001	0.00022	0.00023	1.04231
D77	-3.06280	0.00000	-0.00011	0.00025	0.00013	-3.06266
D78	-0.97570	0.00000	-0.00010	0.00028	0.00018	-0.97553
D79	-3.02384	0.00000	0.00006	0.00022	0.00029	-3.02356
D80	-0.84554	0.00000	-0.00006	0.00025	0.00019	-0.84535
D81	1.24156	0.00000	-0.00005	0.00028	0.00023	1.24179
D82	1.61346	0.00000	-0.00243	-0.00156	-0.00399	1.60947
D83	-1.45154	-0.00001	-0.00249	-0.00140	-0.00389	-1.45543
D84	-0.50704	0.00000	-0.00208	-0.00139	-0.00348	-0.51052
D85	2.71114	0.00000	-0.00215	-0.00123	-0.00338	2.70777
D86	-2.62885	0.00000	-0.00229	-0.00144	-0.00373	-2.63258
D87	0.58934	-0.00001	-0.00235	-0.00128	-0.00363	0.58571
D88	0.09672	0.00000	-0.00011	0.00023	0.00012	0.09684
D89	-3.04547	0.00000	-0.00001	0.00015	0.00013	-3.04534
D90	2.17973	0.00000	-0.00001	0.00016	0.00015	2.17987

This journal is © The Royal Society of Chemistry 2014

D91	-0.96246	0.00000	0.00009	0.00007	0.00016	-0.96230
D92	-2.01249	0.00000	0.00022	0.00021	0.00043	-2.01206
D93	1.12850	0.00000	0.00032	0.00013	0.00045	1.12895
D94	-0.01477	0.00000	-0.00003	-0.00002	-0.00004	-0.01481
D95	3.13782	0.00000	0.00000	0.00002	0.00002	3.13784
D96	3.12139	0.00000	-0.00002	-0.00003	-0.00005	3.12134
D97	-0.00920	0.00000	0.00000	0.00000	0.00001	-0.00920
D98	-3.13751	0.00000	-0.00001	0.00004	0.00003	-3.13748
D99	0.01564	0.00000	0.00007	0.00001	0.00009	0.01573
D100	0.01885	0.00000	0.00003	-0.00007	-0.00004	0.01881
D101	-3.11118	0.00000	0.00011	-0.00010	0.00001	-3.11117
D102	0.00413	0.00000	-0.00003	-0.00002	-0.00005	0.00408
D103	3.13470	0.00000	-0.00005	-0.00006	-0.00011	3.13459
D104	-3.12584	0.00000	0.00006	-0.00005	0.00001	-3.12583
D105	0.00473	0.00000	0.00003	-0.00009	-0.00005	0.00468
D106	-3.13274	0.00000	0.00001	0.00000	0.00001	-3.13274
D107	0.01403	0.00000	-0.00001	0.00005	0.00004	0.01407
D108	0.00650	0.00000	0.00006	-0.00007	-0.00002	0.00648
D109	-3.12992	0.00000	0.00003	-0.00002	0.00002	-3.12990
D110	3.13262	0.00000	0.00001	-0.00005	-0.00004	3.13257
D111	-0.00411	0.00000	0.00006	-0.00010	-0.00004	-0.00415
D112	-0.00378	0.00000	-0.00002	0.00001	-0.00001	-0.00379
D113	-3.14051	0.00000	0.00003	-0.00004	-0.00001	-3.14052
D114	-0.01239	0.00000	-0.00007	0.00008	0.00001	-0.01238
D115	3.11795	0.00000	-0.00002	0.00009	0.00007	3.11802
D116	3.13403	0.00000	-0.00002	0.00004	0.00001	3.13405

This journal is © The Royal Society of Chemistry 2014

```
   D117      -0.01881   0.00000   0.00003   0.00004   0.00007  -
0.01874
   D118       0.00889   0.00000  -0.00019   0.00027   0.00009
0.00898
   D119      -3.12958   0.00000  -0.00024   0.00027   0.00002  -
3.12955
   D120      -0.06852   0.00000   0.00019  -0.00032  -0.00014  -
0.06866
   D121       3.07361   0.00000   0.00010  -0.00025  -0.00015
3.07346
         Item               Value     Threshold  Converged?
 Maximum Force            0.000045     0.000450     YES
 RMS     Force            0.000011     0.000300     YES
 Maximum Displacement     0.007786     0.001800     NO
 RMS     Displacement     0.000763     0.001200     YES
 Predicted change in Energy=-1.325782D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.620081   -1.034052   -0.392832
      2          6           0       -0.184746   -1.436165   -0.666678
      3          1           0       -0.093711   -2.444903   -1.076781
      4          6           0       -1.748838    0.263579    0.133151
      5          6           0        0.337669   -0.373907   -1.701360
      6          1           0       -0.252355   -0.458798   -2.618736
      7          6           0        0.596575   -1.256286    0.622275
      8          6           0        0.479425    0.028482    1.187462
      9          6           0       -0.391861    0.971010    0.348144
     10          6           0        0.281587    1.033365   -1.074179
     11          1           0       -0.262519    1.760250   -1.684817
     12          6           0        1.386443   -2.228305    1.232466
     13          1           0        1.480118   -3.214633    0.784215
     14          6           0        1.172944    0.336044    2.358945
     15          1           0        1.129367    1.329056    2.795642
     16          6           0        1.955948   -0.647434    2.977031
     17          1           0        2.492021   -0.407082    3.891119
     18          6           0        2.061485   -1.923188    2.420230
     19          1           0        2.676136   -2.678399    2.902444
     20          6           0       -2.749229   -1.808342   -0.646418
     21          1           0       -2.642869   -2.809683   -1.057875
     22          6           0       -4.019486   -1.289114   -0.365176
     23          1           0       -4.903835   -1.892014   -0.553325
     24          6           0       -4.149537    0.001688    0.149569
     25          1           0       -5.135690    0.406835    0.359586
     26          6           0       -3.014862    0.787377    0.394349
     27          1           0       -3.136381    1.797408    0.774261
```

28	6	0	1.800882	-0.577040	-2.058094
29	6	0	1.744120	1.467571	-1.009745
30	8	0	2.544254	0.516510	-1.639208
31	8	0	2.220340	2.449996	-0.519046
32	8	0	2.311124	-1.510488	-2.611520
33	6	0	-0.616506	2.360141	0.931882
34	1	0	-0.599310	2.434552	2.036880
35	8	0	-0.881626	3.330409	0.256956

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515543	0.000000			
3	H	2.188171	1.092715	0.000000		
4	C	1.406087	2.444430	3.396948	0.000000	
5	C	2.445572	1.572220	2.205723	2.850497	0.000000
6	H	2.675115	2.184112	2.519406	3.214681	1.094036
7	C	2.448140	1.517965	2.185428	2.837286	2.498981
8	C	2.834471	2.454414	3.401898	2.476287	2.920155
9	C	2.465328	2.620544	3.713188	1.545337	2.557633
10	C	2.890465	2.545997	3.498458	2.484521	1.541726
11	H	3.364568	3.355551	4.252237	2.784632	2.217009
12	C	3.620361	2.588990	2.751435	4.153067	3.625749
13	H	3.968830	2.835457	2.555921	4.790408	3.943729
14	C	4.153363	3.760112	4.598075	3.673721	4.205686
15	H	4.828054	4.621796	5.543857	4.063025	4.873387
16	C	4.928837	4.298986	4.885222	4.758470	4.957922
17	H	5.971156	5.384943	5.959762	5.705874	5.993176
18	C	4.717818	3.848603	4.140790	4.952902	4.728564
19	H	5.658639	4.739876	4.853948	5.992046	5.654567
20	C	1.392411	2.591428	2.764452	2.429273	3.563628
21	H	2.154355	2.842878	2.575195	3.415080	3.902651
22	C	2.413082	3.849384	4.153786	2.795537	4.648418
23	H	3.397779	4.742410	4.870009	3.882246	5.576379
24	C	2.786594	4.295724	4.892798	2.414997	4.868473
25	H	3.873215	5.381609	5.968008	3.397435	5.900400
26	C	2.425422	3.752262	4.598368	1.394778	4.120685
27	H	3.417373	4.609170	5.539079	2.165393	4.786683
28	C	3.832094	2.572324	2.835731	4.255432	1.519708
29	C	4.237516	3.502841	4.323143	3.867371	2.418155
30	O	4.615125	3.493737	4.005640	4.651437	2.380278
31	O	5.186844	4.572579	5.442971	4.578226	3.593988
32	O	4.539156	3.165012	3.001964	5.211893	2.452495
33	C	3.779229	4.141708	5.234166	2.513110	3.914005
34	H	4.356224	4.739571	5.810301	3.107849	4.768629
35	O	4.473931	4.904994	5.979456	3.189488	4.363902

		6	7	8	9	10
6	H	0.000000				
7	C	3.443955	0.000000			
8	C	3.906416	1.408470	0.000000		
9	C	3.296390	2.452143	1.533608	0.000000	
10	C	2.212985	2.866998	2.482730	1.574936	0.000000

This journal is © The Royal Society of Chemistry 2014

11	H	2.407589	3.893611	3.435038	2.184618	1.094208
12	C	4.544070	1.393214	2.432651	3.765635	4.144853
13	H	4.709158	2.154529	3.417864	4.605874	4.789113
14	C	5.238374	2.425642	1.395685	2.625856	3.614846
15	H	5.866948	3.419267	2.167986	2.903891	3.972617
16	C	6.018704	2.786301	2.416515	3.878482	4.694771
17	H	7.064877	3.872881	3.398533	4.771645	5.622730
18	C	5.734934	2.413164	2.798508	4.323058	4.911226
19	H	6.632203	3.397962	3.885088	5.408812	5.943449
20	C	3.456253	3.620601	4.142613	3.777716	4.176617
21	H	3.698311	3.966099	4.779690	4.619260	4.829258
22	C	4.467575	4.720609	4.938313	4.333202	4.939212
23	H	5.287371	5.660450	5.974791	5.419175	5.976432
24	C	4.802456	4.932700	4.743967	3.885762	4.711346
25	H	5.785039	5.974432	5.688413	4.777273	5.638715
26	C	4.273533	4.155837	3.662647	2.629827	3.617134
27	H	4.992044	4.825257	4.046466	2.897740	3.960176
28	C	2.131685	3.015976	3.556197	3.604797	2.422757
29	C	3.207127	3.376351	2.915158	2.579312	1.526987
30	O	3.119571	3.471393	3.534368	3.574480	2.388736
31	O	4.357064	4.204254	3.436086	3.124582	2.464504
32	O	2.770835	3.669023	4.489523	4.714188	3.599115
33	C	4.548177	3.827005	2.589019	1.523450	2.567331
34	H	5.492415	4.129593	2.770263	2.244286	3.523917
35	O	4.798300	4.832836	3.690667	2.411420	2.898516

		11	12	13	14	15
11	H	0.000000				
12	C	5.209432	0.000000			
13	H	5.820856	1.087450	0.000000		
14	C	4.521164	2.808989	3.896336	0.000000	
15	H	4.711453	3.894152	4.981363	1.085669	0.000000
16	C	5.696610	2.422188	3.409599	1.400841	2.150035
17	H	6.586037	3.406991	4.308032	2.154010	2.463954
18	C	5.984991	1.399843	2.163877	2.428454	3.403949
19	H	7.027109	2.157480	2.490964	3.412014	4.296928
20	C	4.471783	4.561837	4.680998	5.386469	6.060904
21	H	5.190704	4.671083	4.533906	6.010881	6.797685
22	C	5.015463	5.714771	5.939223	6.084678	6.584548
23	H	6.013412	6.547499	6.655313	7.097381	7.615144
24	C	4.643966	6.065691	6.514639	5.772516	6.052309
25	H	5.455191	7.088307	7.554089	6.618256	6.784969
26	C	3.583965	5.400765	6.030997	4.647694	4.820193
27	H	3.782529	6.072253	6.814156	4.818412	4.743622
28	C	3.140045	3.704891	3.890824	4.553928	5.257651
29	C	2.137284	4.337619	5.021058	3.599259	3.857212
30	O	3.070333	4.137759	4.574582	4.230636	4.725467
31	O	2.828315	5.064550	5.859560	3.721379	3.665227
32	O	4.263818	4.018274	3.889177	5.423159	6.220688
33	C	2.707820	5.015575	5.957831	3.055423	2.754054
34	H	3.797254	5.131523	6.148698	2.765565	2.187731
35	O	2.572776	6.082356	6.978067	4.195931	3.807156

		16	17	18	19	20

This journal is © The Royal Society of Chemistry 2014

16	C	0.000000				
17	H	1.086601	0.000000			
18	C	1.395963	2.155795	0.000000		
19	H	2.156166	2.484000	1.086586	0.000000	
20	C	6.051098	7.072728	5.706180	6.541101	0.000000
21	H	6.488829	7.525432	5.917266	6.632735	1.087792
22	C	6.876620	7.829033	6.718537	7.578839	1.400802
23	H	7.814667	8.755387	7.573552	8.367599	2.158239
24	C	6.759649	7.633911	6.887513	7.832688	2.422946
25	H	7.632420	8.444890	7.840573	8.775501	3.407969
26	C	5.782550	6.631734	6.100873	7.119663	2.809185
27	H	6.063107	6.800993	6.600747	7.638545	3.894824
28	C	5.038004	5.991636	4.683525	5.457904	4.920614
29	C	4.518020	5.300203	4.833497	5.776066	5.572593
30	O	4.796930	5.607163	4.760696	5.554408	5.866134
31	O	4.678304	5.261773	5.271557	6.181810	6.545707
32	O	5.665944	6.598071	5.054814	5.648102	5.436682
33	C	4.454847	5.106618	5.266281	6.333363	4.941234
34	H	4.112404	4.590144	5.120223	6.133516	5.461172
35	O	5.592305	6.209467	6.398588	7.467399	5.541732

		21	22	23	24	25
21	H	0.000000				
22	C	2.164956	0.000000			
23	H	2.491717	1.086721	0.000000		
24	C	3.410538	1.395724	2.156185	0.000000	
25	H	4.309215	2.155791	2.484325	1.086623	0.000000
26	C	3.896944	2.428572	3.412542	1.401682	2.154979
27	H	4.982525	3.406583	4.300955	2.154376	2.470402
28	C	5.072677	6.103253	6.996193	6.373083	7.411425
29	C	6.127225	6.421365	7.462602	6.182881	7.094506
30	O	6.189326	6.925757	7.902795	6.947777	7.936545
31	O	7.183688	7.275991	8.343147	6.856865	7.684900
32	O	5.351988	6.720988	7.512480	7.186823	8.243703
33	C	5.898505	5.155550	6.218349	4.319332	4.956405
34	H	6.423056	5.597603	6.630028	4.699456	5.244397
35	O	6.521617	5.619004	6.641418	4.665958	5.162837

		26	27	28	29	30
26	C	0.000000				
27	H	1.085938	0.000000			
28	C	5.573823	6.167398	0.000000		
29	C	5.008198	5.206799	2.298411	0.000000	
30	O	5.925580	6.303582	1.387055	1.393181	0.000000
31	O	5.568297	5.549142	3.421632	1.196968	2.257886
32	O	6.533113	7.216717	1.199147	3.428704	2.260191
33	C	2.917986	2.586752	4.838466	3.184204	4.472123
34	H	3.353503	2.904633	5.621336	3.963413	5.203317
35	O	3.322135	2.775179	5.274795	3.459659	4.821838

		31	32	33	34	35
31	O	0.000000				
32	O	4.480192	0.000000			
33	C	3.187626	6.009034	0.000000		
34	H	3.805709	6.755856	1.107634	0.000000	

This journal is © The Royal Society of Chemistry 2014

35 O 3.316550 6.469628 1.211294 2.012558 0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.622513	-1.025588	-0.410336
2	6	0	-0.186586	-1.432037	-0.674504
3	1	0	-0.096285	-2.438451	-1.090439
4	6	0	-1.750312	0.269112	0.123049
5	6	0	0.349191	-0.365277	-1.697657
6	1	0	-0.233272	-0.441639	-2.620597
7	6	0	0.584370	-1.263940	0.622258
8	6	0	0.467786	0.017592	1.194860
9	6	0	-0.392261	0.969310	0.354321
10	6	0	0.293656	1.038089	-1.061734
11	1	0	-0.242103	1.771274	-1.672219
12	6	0	1.364849	-2.243300	1.232791
13	1	0	1.458212	-3.227066	0.778880
14	6	0	1.152494	0.314513	2.374245
15	1	0	1.109354	1.304824	2.817077
16	6	0	1.925993	-0.676329	2.992539
17	1	0	2.455192	-0.444258	3.912752
18	6	0	2.030929	-1.948852	2.428281
19	1	0	2.638216	-2.709824	2.910769
20	6	0	-2.752696	-1.793366	-0.678685
21	1	0	-2.647029	-2.792439	-1.095793
22	6	0	-4.023122	-1.270560	-0.404935
23	1	0	-4.908358	-1.868427	-0.604624
24	6	0	-4.152147	0.017391	0.117157
25	1	0	-5.138352	0.425370	0.321371
26	6	0	-3.016313	0.796601	0.376823
27	1	0	-3.136832	1.804635	0.762315
28	6	0	1.814548	-0.572329	-2.043159
29	6	0	1.757401	1.465603	-0.981906
30	8	0	2.558899	0.515268	-1.610728
31	8	0	2.233525	2.442750	-0.480687
32	8	0	2.325588	-1.504310	-2.598319
33	6	0	-0.616053	2.355540	0.945238
34	1	0	-0.608050	2.422646	2.050809
35	8	0	-0.871258	3.331329	0.274462

Rotational constants (GHZ): 0.3746007 0.2672056 0.2547398
Standard basis: 6-31+G(d) (6D, 7F)
There are 461 symmetry adapted basis functions of A symmetry.

```
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1927.9274045279 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1032.18960853     A.U. after   12 cycles
            Convg  =    0.5192D-08             -V/T =  2.0093
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000012808   -0.000011410   -0.000000527
      2        6          -0.000013514   -0.000006787    0.000008087
      3        1           0.000001220    0.000001839   -0.000001400
      4        6           0.000006140    0.000011988    0.000001195
      5        6          -0.000019821    0.000038525    0.000018706
      6        1           0.000000396    0.000002510   -0.000002154
      7        6           0.000001641   -0.000004250   -0.000011333
      8        6          -0.000013809    0.000012455   -0.000009041
      9        6           0.000005779   -0.000028454    0.000045990
     10        6          -0.000001438   -0.000019873   -0.000051771
     11        1          -0.000000769    0.000003151    0.000005589
     12        6           0.000001701   -0.000001065   -0.000002272
     13        1          -0.000000204   -0.000002055   -0.000002891
     14        6           0.000005554   -0.000004029    0.000006505
     15        1           0.000000064   -0.000000440   -0.000003710
     16        6           0.000004058    0.000001574   -0.000001339
     17        1           0.000004137   -0.000004943   -0.000003015
     18        6           0.000001424   -0.000003303   -0.000004559
     19        1           0.000002260   -0.000003845   -0.000005219
     20        6          -0.000005171    0.000006858    0.000001766
     21        1          -0.000002540   -0.000000172    0.000001358
     22        6          -0.000000365   -0.000001821   -0.000000687
     23        1          -0.000001150    0.000001512    0.000002244
     24        6          -0.000001291    0.000008714    0.000007537
     25        1           0.000000255    0.000000673    0.000004267
     26        6          -0.000003494   -0.000001958   -0.000001578
     27        1           0.000002407    0.000001962    0.000007261
     28        6           0.000012964   -0.000027092   -0.000030623
     29        6           0.000018177   -0.000009844    0.000005849
     30        8          -0.000008041    0.000018861    0.000002946
     31        8           0.000001723    0.000002968   -0.000003507
     32        8          -0.000007076    0.000011128    0.000011985
     33        6          -0.000017877    0.000042891   -0.000030586
     34        1           0.000002422   -0.000012433    0.000010665
```

```
     35        8           0.000011427   -0.000023834    0.000024263
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000051771 RMS     0.000013096


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000033147 RMS     0.000004928
 Search for a local minimum.
 Step number   9 out of a maximum of  210
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8    9
 DE=  2.00D-07 DEPred=-1.33D-07 R=-1.51D+00
 Trust test=-1.51D+00 RLast= 9.38D-03 DXMaxT set to 5.00D-02
     Eigenvalues ---    0.00159   0.00486   0.01088   0.01121
0.01164
     Eigenvalues ---    0.01429   0.01486   0.01628   0.01802
0.02032
     Eigenvalues ---    0.02115   0.02121   0.02131   0.02132
0.02136
     Eigenvalues ---    0.02139   0.02144   0.02146   0.02158
0.02160
     Eigenvalues ---    0.02166   0.02179   0.02804   0.03853
0.03970
     Eigenvalues ---    0.04649   0.04877   0.04942   0.05279
0.05344
     Eigenvalues ---    0.05478   0.05721   0.06293   0.06596
0.08308
     Eigenvalues ---    0.09075   0.09409   0.09998   0.12419
0.15424
     Eigenvalues ---    0.15943   0.15999   0.16000   0.16000
0.16001
     Eigenvalues ---    0.16002   0.16003   0.16045   0.16620
0.20316
     Eigenvalues ---    0.20848   0.21996   0.22002   0.22125
0.22609
     Eigenvalues ---    0.22688   0.22793   0.24209   0.24589
0.24616
     Eigenvalues ---    0.24759   0.25050   0.26685   0.27452
0.28549
     Eigenvalues ---    0.28799   0.28833   0.29806   0.30411
0.30999
     Eigenvalues ---    0.32542   0.34386   0.34420   0.34531
0.35127
     Eigenvalues ---    0.35169   0.35233   0.35244   0.35248
0.35304
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.35349   0.35438   0.36721   0.40018
0.42024
     Eigenvalues ---    0.42102   0.43400   0.43704   0.44196
0.44819
     Eigenvalues ---    0.46054   0.46219   0.46328   0.46466
0.46815
     Eigenvalues ---    0.48902   0.98884   1.05131
1.059921000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     9    8    7    6
5
 RFO step:  Lambda=-1.12060831D-08.
 DIIS coeffs:      1.37891     -0.52721      0.12191      0.01249
0.01391
 Iteration  1 RMS(Cart)=  0.00033514 RMS(Int)=  0.00000019
 Iteration  2 RMS(Cart)=  0.00000020 RMS(Int)=  0.00000001
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86396  -0.00001  -0.00002   0.00000  -0.00002
2.86394
    R2        2.65712   0.00000   0.00001  -0.00001   0.00001
2.65713
    R3        2.63128   0.00000   0.00001   0.00000   0.00000
2.63128
    R4        2.06493   0.00000   0.00000  -0.00001   0.00000
2.06493
    R5        2.97107   0.00001   0.00000   0.00004   0.00004
2.97110
    R6        2.86854   0.00000   0.00001  -0.00002  -0.00001
2.86853
    R7        2.92026  -0.00001   0.00003  -0.00005  -0.00002
2.92024
    R8        2.63575   0.00000   0.00002  -0.00001   0.00001
2.63576
    R9        2.06743   0.00000  -0.00001   0.00000   0.00000
2.06742
   R10        2.91344  -0.00002   0.00002  -0.00007  -0.00005
2.91339
   R11        2.87183   0.00002   0.00003   0.00003   0.00006
2.87189
   R12        2.66162   0.00000   0.00001  -0.00001   0.00000
2.66163
   R13        2.63279   0.00000   0.00001   0.00000   0.00001
2.63280
   R14        2.89810  -0.00002  -0.00001  -0.00005  -0.00006
2.89804
   R15        2.63746   0.00000   0.00001   0.00000   0.00000
2.63746
   R16        2.97620   0.00003  -0.00001   0.00009   0.00008
2.97628
   R17        2.87890   0.00001   0.00000  -0.00001   0.00000
2.87890
```

This journal is © The Royal Society of Chemistry 2014

R18	2.06775	0.00000	0.00000	0.00000	0.00000
2.06775					
R19	2.88559	0.00001	0.00005	0.00001	0.00006
2.88565					
R20	2.05498	0.00000	0.00000	0.00000	0.00000
2.05498					
R21	2.64532	0.00000	0.00001	-0.00001	0.00000
2.64532					
R22	2.05162	0.00000	0.00001	0.00000	0.00000
2.05162					
R23	2.64721	0.00000	0.00001	-0.00001	0.00000
2.64721					
R24	2.05338	0.00000	0.00000	0.00000	0.00000
2.05338					
R25	2.63799	0.00000	0.00001	-0.00001	0.00001
2.63800					
R26	2.05335	0.00000	0.00000	0.00000	0.00000
2.05335					
R27	2.05563	0.00000	0.00000	0.00000	0.00000
2.05563					
R28	2.64713	0.00000	0.00001	-0.00001	0.00000
2.64714					
R29	2.05361	0.00000	0.00000	0.00000	0.00000
2.05361					
R30	2.63754	0.00000	0.00001	0.00000	0.00001
2.63754					
R31	2.05342	0.00000	0.00000	0.00000	0.00000
2.05342					
R32	2.64880	0.00000	0.00001	-0.00002	0.00000
2.64879					
R33	2.05213	0.00000	0.00001	0.00000	0.00001
2.05214					
R34	2.62115	0.00001	-0.00006	0.00001	-0.00005
2.62110					
R35	2.26606	-0.00002	0.00002	-0.00002	0.00000
2.26606					
R36	2.63273	-0.00001	0.00007	-0.00002	0.00005
2.63278					
R37	2.26194	0.00000	-0.00002	-0.00001	-0.00002
2.26192					
R38	2.09312	0.00001	0.00003	0.00002	0.00005
2.09318					
R39	2.28901	-0.00003	-0.00002	-0.00003	-0.00005
2.28896					
A1	1.98142	0.00000	-0.00001	-0.00001	-0.00002
1.98140					
A2	2.19884	0.00001	0.00002	0.00002	0.00004
2.19888					
A3	2.10256	-0.00001	-0.00001	-0.00002	-0.00003
2.10253					
A4	1.97322	0.00000	0.00000	0.00003	0.00004
1.97326					

This journal is © The Royal Society of Chemistry 2014

A5	1.82796	0.00000	-0.00003	0.00001	-0.00002
1.82794					
A6	1.87822	0.00000	0.00001	0.00003	0.00004
1.87826					
A7	1.92735	0.00000	0.00001	-0.00003	-0.00001
1.92734					
A8	1.96622	0.00000	-0.00001	-0.00001	-0.00002
1.96620					
A9	1.88360	0.00000	0.00001	-0.00004	-0.00003
1.88357					
A10	1.97589	0.00000	0.00001	-0.00001	0.00001
1.97590					
A11	2.09410	0.00000	0.00000	0.00002	0.00002
2.09412					
A12	2.21315	0.00000	-0.00001	-0.00001	-0.00002
2.21313					
A13	1.89675	0.00000	0.00000	0.00001	0.00001
1.89676					
A14	1.91443	0.00000	0.00002	0.00002	0.00004
1.91447					
A15	1.96503	0.00000	-0.00003	-0.00004	-0.00007
1.96496					
A16	1.97395	0.00000	0.00000	0.00000	0.00000
1.97396					
A17	1.88815	0.00000	0.00000	-0.00001	-0.00001
1.88815					
A18	1.82609	0.00000	0.00001	0.00001	0.00002
1.82611					
A19	1.98889	0.00000	0.00001	-0.00002	-0.00001
1.98887					
A20	2.19080	0.00001	0.00002	0.00002	0.00004
2.19084					
A21	2.10344	0.00000	-0.00003	0.00000	-0.00003
2.10341					
A22	1.96953	0.00000	0.00000	0.00001	0.00001
1.96953					
A23	2.09036	0.00000	0.00003	0.00000	0.00003
2.09039					
A24	2.22212	0.00000	-0.00003	-0.00001	-0.00005
2.22207					
A25	1.86886	0.00000	0.00000	0.00003	0.00003
1.86889					
A26	1.84208	0.00000	0.00003	-0.00006	-0.00003
1.84205					
A27	1.91904	0.00000	-0.00010	-0.00005	-0.00015
1.91889					
A28	1.85006	0.00000	-0.00003	0.00006	0.00003
1.85009					
A29	2.02024	0.00000	-0.00007	0.00000	-0.00007
2.02018					
A30	1.95303	0.00001	0.00017	0.00002	0.00019
1.95322					

This journal is © The Royal Society of Chemistry 2014

A31	1.92495	0.00000	-0.00003	-0.00003	-0.00005
1.92490					
A32	1.97952	0.00000	-0.00002	0.00003	0.00001
1.97953					
A33	1.81510	0.00000	-0.00002	0.00002	0.00000
1.81510					
A34	1.89405	0.00000	0.00004	0.00000	0.00004
1.89409					
A35	1.96352	0.00000	0.00006	0.00001	0.00006
1.96358					
A36	1.88696	0.00000	-0.00004	-0.00002	-0.00006
1.88690					
A37	2.09567	0.00000	0.00000	0.00001	0.00001
2.09568					
A38	2.08627	0.00000	0.00000	0.00000	0.00000
2.08627					
A39	2.10123	0.00000	0.00000	-0.00001	-0.00001
2.10122					
A40	2.11675	-0.00001	-0.00002	-0.00003	-0.00006
2.11670					
A41	2.08677	0.00000	-0.00001	0.00001	-0.00001
2.08676					
A42	2.07957	0.00000	0.00004	0.00002	0.00006
2.07963					
A43	2.08477	0.00000	0.00001	0.00001	0.00002
2.08479					
A44	2.10351	0.00000	-0.00001	0.00000	-0.00002
2.10350					
A45	2.09485	0.00000	0.00000	-0.00001	-0.00001
2.09484					
A46	2.09575	0.00000	0.00002	0.00000	0.00002
2.09577					
A47	2.09191	0.00000	-0.00001	-0.00001	-0.00002
2.09189					
A48	2.09547	0.00000	-0.00001	0.00000	0.00000
2.09547					
A49	2.09611	0.00000	0.00000	0.00000	0.00000
2.09611					
A50	2.08596	0.00000	0.00000	0.00001	0.00002
2.08597					
A51	2.10112	0.00000	-0.00001	-0.00001	-0.00002
2.10110					
A52	2.09155	0.00000	0.00000	-0.00001	-0.00001
2.09154					
A53	2.09594	0.00000	0.00001	0.00000	0.00001
2.09595					
A54	2.09568	0.00000	0.00000	0.00000	0.00000
2.09568					
A55	2.09516	0.00000	0.00000	0.00000	0.00000
2.09516					
A56	2.10293	0.00000	-0.00001	-0.00001	-0.00002
2.10291					

This journal is © The Royal Society of Chemistry 2014

A57	2.08508	0.00000	0.00001	0.00001	0.00002	2.08510
A58	2.08469	0.00000	0.00001	0.00000	0.00001	2.08470
A59	2.11341	0.00000	0.00000	-0.00001	-0.00001	2.11341
A60	2.08502	0.00000	-0.00001	0.00001	0.00000	2.08502
A61	1.91744	-0.00001	0.00001	-0.00002	-0.00001	1.91742
A62	2.24218	0.00001	-0.00003	0.00001	-0.00002	2.24216
A63	2.12356	0.00000	0.00003	0.00001	0.00004	2.12360
A64	1.91442	0.00000	-0.00002	-0.00001	-0.00003	1.91439
A65	2.25460	0.00000	0.00006	-0.00001	0.00006	2.25466
A66	2.11416	0.00000	-0.00005	0.00001	-0.00003	2.11413
A67	1.94642	0.00000	0.00001	0.00001	0.00002	1.94644
A68	2.02776	-0.00002	-0.00013	-0.00011	-0.00024	2.02752
A69	2.15217	0.00001	0.00011	0.00004	0.00016	2.15232
A70	2.10070	0.00001	0.00002	0.00006	0.00008	2.10078
D1	-3.13980	0.00000	-0.00001	0.00008	0.00007	-3.13974
D2	-1.04056	0.00000	-0.00001	0.00007	0.00006	-1.04050
D3	0.96075	0.00000	-0.00001	0.00005	0.00004	0.96079
D4	-0.02745	0.00000	-0.00004	-0.00008	-0.00012	-0.02757
D5	2.07180	0.00000	-0.00005	-0.00008	-0.00013	2.07167
D6	-2.21008	0.00000	-0.00004	-0.00011	-0.00015	-2.21023
D7	-0.02716	0.00000	0.00001	-0.00012	-0.00011	-0.02727
D8	3.10510	0.00000	-0.00004	-0.00014	-0.00017	3.10493
D9	-3.14131	0.00000	0.00004	0.00003	0.00006	-3.14124
D10	-0.00905	0.00000	-0.00001	0.00001	0.00000	-0.00905
D11	0.02595	0.00000	0.00005	0.00014	0.00019	0.02614
D12	-3.11800	0.00000	0.00003	0.00019	0.00022	-3.11778

This journal is © The Royal Society of Chemistry 2014

D13	3.13645	0.00000	0.00002	-0.00003	-0.00001	3.13644
D14	-0.00751	0.00000	0.00000	0.00003	0.00002	-0.00749
D15	-1.09445	0.00000	0.00010	-0.00008	0.00002	-1.09443
D16	1.07169	0.00000	0.00011	-0.00005	0.00006	1.07175
D17	3.09736	0.00000	0.00012	-0.00005	0.00007	3.09743
D18	1.03507	0.00000	0.00009	-0.00004	0.00005	1.03512
D19	-3.08197	0.00000	0.00010	-0.00001	0.00008	-3.08189
D20	-1.05630	0.00000	0.00011	-0.00002	0.00009	-1.05621
D21	-3.09199	0.00000	0.00010	-0.00010	0.00000	-3.09199
D22	-0.92584	0.00000	0.00011	-0.00007	0.00003	-0.92581
D23	1.09983	0.00000	0.00012	-0.00008	0.00004	1.09987
D24	-0.93651	0.00000	-0.00002	0.00012	0.00009	-0.93642
D25	2.21697	0.00000	0.00003	0.00010	0.00013	2.21709
D26	-3.12334	0.00000	-0.00002	0.00006	0.00003	-3.12331
D27	0.03014	0.00000	0.00002	0.00004	0.00007	0.03021
D28	1.02748	0.00000	-0.00005	0.00012	0.00008	1.02755
D29	-2.10223	0.00000	0.00000	0.00011	0.00011	-2.10212
D30	-0.92289	0.00000	0.00000	0.00008	0.00008	-0.92281
D31	1.04286	0.00000	-0.00002	0.00013	0.00011	1.04297
D32	-3.13104	0.00000	0.00015	0.00009	0.00024	-3.13079
D33	2.22880	0.00000	0.00005	0.00010	0.00015	2.22895
D34	-2.08864	0.00000	0.00003	0.00015	0.00018	-2.08846
D35	0.02066	0.00000	0.00020	0.00011	0.00031	0.02096
D36	0.01889	0.00000	0.00000	-0.00001	-0.00001	0.01888
D37	-3.11132	0.00000	-0.00001	-0.00004	-0.00006	-3.11138
D38	-3.13341	0.00000	-0.00005	-0.00003	-0.00009	-3.13350

This journal is © The Royal Society of Chemistry 2014

D39	0.01956	0.00000	-0.00006	-0.00007	-0.00013	0.01943
D40	-0.08376	0.00000	-0.00013	0.00007	-0.00006	-0.08382
D41	-2.21224	0.00000	-0.00015	0.00007	-0.00008	-2.21232
D42	2.02534	0.00000	-0.00009	0.00007	-0.00001	2.02533
D43	2.03665	0.00000	-0.00012	0.00010	-0.00001	2.03663
D44	-0.09183	0.00000	-0.00014	0.00010	-0.00004	-0.09186
D45	-2.13743	0.00000	-0.00008	0.00011	0.00003	-2.13740
D46	-2.19557	0.00000	-0.00011	0.00010	-0.00001	-2.19557
D47	1.95914	0.00000	-0.00013	0.00011	-0.00003	1.95911
D48	-0.08646	0.00000	-0.00007	0.00011	0.00004	-0.08642
D49	-2.02567	0.00000	0.00000	-0.00015	-0.00015	-2.02582
D50	1.11260	-0.00001	-0.00009	-0.00018	-0.00027	1.11233
D51	2.16118	0.00000	0.00003	-0.00014	-0.00011	2.16107
D52	-0.98374	0.00000	-0.00007	-0.00016	-0.00023	-0.98397
D53	0.05229	0.00000	0.00002	-0.00015	-0.00013	0.05217
D54	-3.09263	0.00000	-0.00007	-0.00017	-0.00024	-3.09287
D55	-0.02335	0.00000	0.00002	-0.00015	-0.00013	-0.02348
D56	-3.11642	0.00000	0.00003	0.00002	0.00004	-3.11637
D57	3.10701	0.00000	-0.00003	-0.00014	-0.00016	3.10685
D58	0.01394	0.00000	-0.00002	0.00003	0.00001	0.01396
D59	-0.00135	0.00000	-0.00002	-0.00002	-0.00004	-0.00139
D60	3.13482	0.00000	-0.00003	-0.00005	-0.00007	3.13475
D61	-3.13033	0.00000	0.00003	-0.00004	-0.00001	-3.13034
D62	0.00584	0.00000	0.00003	-0.00006	-0.00004	0.00580
D63	0.94725	0.00000	-0.00003	0.00008	0.00006	0.94730
D64	-1.01304	0.00000	-0.00005	0.00011	0.00006	-1.01298

This journal is © The Royal Society of Chemistry 2014

D65	3.09389	0.00000	-0.00020	0.00004	-0.00016	3.09373
D66	-2.24731	0.00000	-0.00003	-0.00010	-0.00013	-2.24744
D67	2.07558	0.00000	-0.00005	-0.00007	-0.00013	2.07545
D68	-0.10067	0.00000	-0.00021	-0.00014	-0.00035	-0.10102
D69	3.10201	0.00000	0.00003	-0.00011	-0.00007	3.10193
D70	-0.02457	0.00000	0.00000	0.00002	0.00002	-0.02455
D71	0.01665	0.00000	0.00004	0.00009	0.00013	0.01678
D72	-3.10993	0.00000	0.00001	0.00022	0.00022	-3.10970
D73	-0.93658	0.00000	0.00011	-0.00010	0.00001	-0.93658
D74	1.24163	0.00000	0.00010	-0.00008	0.00001	1.24164
D75	-2.95442	0.00000	0.00012	-0.00011	0.00001	-2.95441
D76	1.04231	0.00000	0.00011	-0.00007	0.00004	1.04235
D77	-3.06266	0.00000	0.00010	-0.00005	0.00005	-3.06262
D78	-0.97553	0.00000	0.00012	-0.00008	0.00004	-0.97549
D79	-3.02356	0.00000	0.00011	-0.00001	0.00010	-3.02346
D80	-0.84535	0.00000	0.00010	0.00000	0.00011	-0.84524
D81	1.24179	0.00000	0.00012	-0.00002	0.00010	1.24189
D82	1.60947	0.00000	-0.00100	-0.00051	-0.00151	1.60795
D83	-1.45543	0.00000	-0.00098	-0.00045	-0.00143	-1.45687
D84	-0.51052	0.00000	-0.00087	-0.00051	-0.00138	-0.51190
D85	2.70777	0.00000	-0.00086	-0.00045	-0.00130	2.70646
D86	-2.63258	0.00000	-0.00092	-0.00061	-0.00153	-2.63410
D87	0.58571	0.00000	-0.00091	-0.00054	-0.00145	0.58426
D88	0.09684	0.00000	0.00010	-0.00004	0.00006	0.09690
D89	-3.04534	0.00000	0.00001	-0.00006	-0.00005	-3.04539
D90	2.17987	0.00000	0.00008	-0.00006	0.00002	2.17990

This journal is © The Royal Society of Chemistry 2014

D91	-0.96230	0.00000	-0.00001	-0.00008	-0.00008	-0.96239
D92	-2.01206	0.00000	0.00015	-0.00007	0.00007	-2.01198
D93	1.12895	0.00000	0.00006	-0.00009	-0.00003	1.12892
D94	-0.01481	0.00000	-0.00001	0.00003	0.00002	-0.01479
D95	3.13784	0.00000	0.00001	0.00003	0.00004	3.13788
D96	3.12134	0.00000	-0.00001	0.00001	-0.00001	3.12133
D97	-0.00920	0.00000	0.00000	0.00001	0.00001	-0.00919
D98	-3.13748	0.00000	0.00001	-0.00006	-0.00005	-3.13752
D99	0.01573	0.00000	0.00002	-0.00005	-0.00004	0.01569
D100	0.01881	0.00000	-0.00002	0.00007	0.00005	0.01886
D101	-3.11117	0.00000	-0.00002	0.00008	0.00006	-3.11111
D102	0.00408	0.00000	-0.00001	0.00002	0.00001	0.00409
D103	3.13459	0.00000	-0.00003	0.00002	0.00000	3.13459
D104	-3.12583	0.00000	-0.00001	0.00003	0.00002	-3.12581
D105	0.00468	0.00000	-0.00003	0.00003	0.00001	0.00468
D106	-3.13274	0.00000	0.00000	-0.00003	-0.00003	-3.13277
D107	0.01407	0.00000	0.00002	-0.00005	-0.00004	0.01403
D108	0.00648	0.00000	-0.00002	0.00002	0.00001	0.00649
D109	-3.12990	0.00000	0.00000	0.00000	0.00000	-3.12990
D110	3.13257	0.00000	-0.00002	0.00003	0.00001	3.13258
D111	-0.00415	0.00000	-0.00003	0.00005	0.00002	-0.00413
D112	-0.00379	0.00000	0.00000	0.00000	0.00000	-0.00379
D113	-3.14052	0.00000	-0.00001	0.00003	0.00001	-3.14050
D114	-0.01238	0.00000	0.00002	-0.00002	0.00000	-0.01238
D115	3.11802	0.00000	0.00003	0.00001	0.00004	3.11806
D116	3.13405	0.00000	0.00001	0.00001	0.00002	3.13406

This journal is © The Royal Society of Chemistry 2014

```
   D117      -0.01874   0.00000   0.00002   0.00004   0.00006  -
0.01868
   D118       0.00898   0.00000   0.00004   0.00013   0.00017
0.00915
   D119      -3.12955   0.00000   0.00013   0.00015   0.00028  -
3.12927
   D120      -0.06866   0.00000  -0.00009  -0.00005  -0.00015  -
0.06880
   D121       3.07346   0.00000  -0.00001  -0.00004  -0.00005
3.07342
         Item               Value     Threshold  Converged?
 Maximum Force            0.000033     0.000450     YES
 RMS     Force            0.000005     0.000300     YES
 Maximum Displacement     0.003173     0.001800     NO
 RMS     Displacement     0.000335     0.001200     YES
 Predicted change in Energy=-2.316458D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.620118   -1.034121   -0.392713
      2          6           0       -0.184794   -1.436219   -0.666578
      3          1           0       -0.093717   -2.444951   -1.076684
      4          6           0       -1.748858    0.263548    0.133190
      5          6           0        0.337569   -0.373936   -1.701290
      6          1           0       -0.252488   -0.458820   -2.618644
      7          6           0        0.596603   -1.256313    0.622321
      8          6           0        0.479376    0.028435    1.187540
      9          6           0       -0.391882    0.970943    0.348228
     10          6           0        0.281569    1.033327   -1.074141
     11          1           0       -0.262492    1.760242   -1.684780
     12          6           0        1.386641   -2.228237    1.232450
     13          1           0        1.480395   -3.214563    0.784209
     14          6           0        1.172973    0.336096    2.358952
     15          1           0        1.129332    1.329146    2.795563
     16          6           0        1.956180   -0.647277    2.976948
     17          1           0        2.492360   -0.406866    3.890957
     18          6           0        2.061789   -1.923022    2.420131
     19          1           0        2.676597   -2.678159    2.902263
     20          6           0       -2.749307   -1.808326   -0.646385
     21          1           0       -2.642992   -2.809695   -1.057787
     22          6           0       -4.019561   -1.288977   -0.365343
     23          1           0       -4.903929   -1.891819   -0.553591
     24          6           0       -4.149589    0.001858    0.149337
     25          1           0       -5.135740    0.407086    0.359202
     26          6           0       -3.014876    0.787458    0.394218
     27          1           0       -3.136350    1.797506    0.774116
```

This journal is © The Royal Society of Chemistry 2014

28	6	0	1.800786	-0.577178	-2.058079
29	6	0	1.744153	1.467492	-1.009806
30	8	0	2.544190	0.516391	-1.639388
31	8	0	2.220494	2.449901	-0.519219
32	8	0	2.310958	-1.510783	-2.611302
33	6	0	-0.616727	2.359946	0.932189
34	1	0	-0.600989	2.433663	2.037282
35	8	0	-0.880562	3.330662	0.257451

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515533	0.000000			
3	H	2.188186	1.092713	0.000000		
4	C	1.406092	2.444409	3.396948	0.000000	
5	C	2.445558	1.572239	2.205730	2.850417	0.000000
6	H	2.675098	2.184136	2.519438	3.214580	1.094034
7	C	2.448166	1.517962	2.185411	2.837326	2.498971
8	C	2.834448	2.454401	3.401879	2.476279	2.920162
9	C	2.465327	2.620524	3.713167	1.545326	2.557601
10	C	2.890518	2.546027	3.498466	2.484520	1.541701
11	H	3.364677	3.355613	4.252284	2.784670	2.216995
12	C	3.620451	2.589017	2.751458	4.153158	3.625716
13	H	3.968961	2.835515	2.555983	4.790528	3.943718
14	C	4.153374	3.760115	4.598078	3.673742	4.205664
15	H	4.828003	4.621752	5.543821	4.062968	4.873301
16	C	4.928911	4.299009	4.885247	4.758557	4.957875
17	H	5.971244	5.384965	5.959785	5.705980	5.993116
18	C	4.717909	3.848621	4.140812	4.953001	4.728500
19	H	5.658753	4.739894	4.853971	5.992166	5.654484
20	C	1.392412	2.591448	2.764527	2.429259	3.563580
21	H	2.154358	2.842925	2.575306	3.415074	3.902661
22	C	2.413095	3.849398	4.153858	2.795525	4.648293
23	H	3.397785	4.742423	4.870085	3.882235	5.576243
24	C	2.786628	4.295740	4.892862	2.415005	4.868329
25	H	3.873249	5.381623	5.968072	3.397448	5.900232
26	C	2.425440	3.752251	4.598390	1.394782	4.120543
27	H	3.417391	4.609149	5.539090	2.165397	4.786534
28	C	3.832077	2.572304	2.835639	4.255402	1.519740
29	C	4.237593	3.502881	4.323130	3.867434	2.418158
30	O	4.615165	3.493766	4.005589	4.651476	2.380272
31	O	5.186976	4.572642	5.442970	4.578377	3.593989
32	O	4.539019	3.164851	3.001697	5.211774	2.452510
33	C	3.779133	4.141677	5.234132	2.512967	3.914077
34	H	4.355345	4.739205	5.809904	3.106858	4.768692
35	O	4.474482	4.905209	5.979694	3.190073	4.364007

		6	7	8	9	10
6	H	0.000000				
7	C	3.443952	0.000000			
8	C	3.906414	1.408471	0.000000		
9	C	3.296358	2.452122	1.533577	0.000000	
10	C	2.212964	2.866998	2.482767	1.574979	0.000000

This journal is © The Royal Society of Chemistry 2014

11	H	2.407580	3.893632	3.435076	2.184686	1.094207
12	C	4.544062	1.393217	2.432635	3.765601	4.144797
13	H	4.709183	2.154539	3.417858	4.605862	4.789072
14	C	5.238348	2.425666	1.395686	2.625798	3.614811
15	H	5.866846	3.419266	2.167956	2.903765	3.972508
16	C	6.018669	2.786331	2.416509	3.878428	4.694685
17	H	7.064828	3.872910	3.398538	4.771598	5.622628
18	C	5.734894	2.413169	2.798481	4.322999	4.911121
19	H	6.632150	3.397963	3.885062	5.408753	5.943321
20	C	3.456165	3.620698	4.142627	3.777703	4.176622
21	H	3.698297	3.966200	4.779713	4.619264	4.829301
22	C	4.467366	4.720754	4.938365	4.333182	4.939150
23	H	5.287138	5.660609	5.974854	5.419156	5.976357
24	C	4.802222	4.932854	4.744037	3.885749	4.711261
25	H	5.784765	5.974604	5.688501	4.777263	5.638607
26	C	4.273328	4.155937	3.662686	2.629805	3.617053
27	H	4.991842	4.825328	4.046480	2.897704	3.960075
28	C	2.131707	3.015928	3.556252	3.604828	2.422783
29	C	3.207119	3.376363	2.915283	2.579431	1.527020
30	O	3.119517	3.471441	3.534555	3.574599	2.388762
31	O	4.357050	4.204303	3.436280	3.124787	2.464559
32	O	2.770908	3.668799	4.489441	4.714141	3.599135
33	C	4.548244	3.826946	2.588936	1.523448	2.567530
34	H	5.492318	4.129439	2.770266	2.244144	3.524316
35	O	4.798601	4.832752	3.690420	2.411498	2.898523

		11	12	13	14	15
11	H	0.000000				
12	C	5.209399	0.000000			
13	H	5.820846	1.087451	0.000000		
14	C	4.521119	2.808997	3.896345	0.000000	
15	H	4.711315	3.894163	4.981374	1.085671	0.000000
16	C	5.696522	2.422206	3.409609	1.400841	2.150076
17	H	6.585925	3.407002	4.308030	2.154023	2.464036
18	C	5.984898	1.399845	2.163871	2.428446	3.403972
19	H	7.026992	2.157473	2.490940	3.412009	4.296965
20	C	4.471822	4.562063	4.681291	5.386546	6.060905
21	H	5.190783	4.671320	4.534224	6.010965	6.797701
22	C	5.015398	5.715083	5.939601	6.084821	6.584602
23	H	6.013325	6.547854	6.655746	7.097553	7.615228
24	C	4.643858	6.065995	6.514993	5.772676	6.052372
25	H	5.455038	7.088649	7.554483	6.618451	6.785070
26	C	3.583874	5.400963	6.031229	4.647793	4.820201
27	H	3.782408	6.072407	6.814343	4.818474	4.743590
28	C	3.140064	3.704739	3.890636	4.553941	5.257639
29	C	2.137269	4.337504	5.020926	3.599282	3.857199
30	O	3.070292	4.137675	4.574440	4.230776	4.725589
31	O	2.828318	5.064448	5.859422	3.721470	3.665312
32	O	4.263882	4.017901	3.888727	5.423043	6.220581
33	C	2.708071	5.015482	5.957765	3.055265	2.753803
34	H	3.797607	5.131446	6.148562	2.765900	2.188369
35	O	2.573031	6.082120	6.977934	4.195323	3.806278

		16	17	18	19	20

16	C	0.000000				
17	H	1.086600	0.000000			
18	C	1.395967	2.155795	0.000000		
19	H	2.156168	2.483995	1.086588	0.000000	
20	C	6.051296	7.072951	5.706428	6.541403	0.000000
21	H	6.489031	7.525656	5.917522	6.633048	1.087794
22	C	6.876929	7.829388	6.718905	7.579288	1.400804
23	H	7.815029	8.755809	7.573983	8.368132	2.158235
24	C	6.759968	7.634283	6.887879	7.833129	2.422958
25	H	7.632797	8.445337	7.840998	8.776018	3.407978
26	C	5.782763	6.631986	6.101110	7.119947	2.809176
27	H	6.063274	6.801201	6.600934	7.638778	3.894823
28	C	5.037912	5.991520	4.683351	5.457669	4.920564
29	C	4.517899	5.300048	4.833316	5.775825	5.572634
30	O	4.796920	5.607121	4.760582	5.554212	5.866130
31	O	4.678201	5.261624	5.271378	6.181551	6.545808
32	O	5.665690	6.597796	5.054438	5.647642	5.436517
33	C	4.454692	5.106465	5.266140	6.333220	4.941081
34	H	4.112697	4.590592	5.120319	6.133636	5.460019
35	O	5.591669	6.208711	6.398110	7.466883	5.542411

		21	22	23	24	25
21	H	0.000000				
22	C	2.164949	0.000000			
23	H	2.491695	1.086722	0.000000		
24	C	3.410544	1.395727	2.156189	0.000000	
25	H	4.309214	2.155794	2.484329	1.086622	0.000000
26	C	3.896938	2.428560	3.412535	1.401681	2.154988
27	H	4.982527	3.406582	4.300961	2.154381	2.470422
28	C	5.072660	6.103150	6.996068	6.372984	7.411303
29	C	6.127290	6.421359	7.462580	6.182871	7.094475
30	O	6.189344	6.925704	7.902716	6.947731	7.936475
31	O	7.183795	7.276069	8.343209	6.856956	7.684979
32	O	5.351841	6.720788	7.512253	7.186645	8.243508
33	C	5.898385	5.155337	6.218131	4.319091	4.956153
34	H	6.421996	5.596185	6.628553	4.697933	5.242798
35	O	6.522269	5.619808	6.642257	4.666815	5.163738

		26	27	28	29	30
26	C	0.000000				
27	H	1.085945	0.000000			
28	C	5.573741	6.167314	0.000000		
29	C	5.008202	5.206784	2.298425	0.000000	
30	O	5.925559	6.303554	1.387028	1.393207	0.000000
31	O	5.568410	5.549245	3.421616	1.196956	2.257879
32	O	6.532959	7.216577	1.199145	3.428728	2.260188
33	C	2.917747	2.586469	4.838674	3.184584	4.472483
34	H	3.352089	2.903160	5.621892	3.964584	5.204420
35	O	3.322933	2.775984	5.274706	3.459259	4.821519

		31	32	33	34	35
31	O	0.000000				
32	O	4.480180	0.000000			
33	C	3.188182	6.009177	0.000000		
34	H	3.807457	6.756287	1.107661	0.000000	

35 O 3.315948 6.469554 1.211268 2.012602 0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.622627	-1.025893	-0.409501
2	6	0	-0.186729	-1.432502	-0.673520
3	1	0	-0.096418	-2.439170	-1.088835
4	6	0	-1.750366	0.269180	0.123005
5	6	0	0.348941	-0.366359	-1.697401
6	1	0	-0.233611	-0.443285	-2.620236
7	6	0	0.584383	-1.263573	0.623036
8	6	0	0.467765	0.018297	1.194877
9	6	0	-0.392298	0.969476	0.353802
10	6	0	0.293538	1.037394	-1.062382
11	1	0	-0.242209	1.770233	-1.673294
12	6	0	1.365063	-2.242463	1.234073
13	1	0	1.458470	-3.226511	0.780781
14	6	0	1.152626	0.316048	2.373965
15	1	0	1.109456	1.306674	2.816095
16	6	0	1.926359	-0.674308	2.992742
17	1	0	2.455724	-0.441608	3.912701
18	6	0	2.031324	-1.947176	2.429258
19	1	0	2.638793	-2.707777	2.912104
20	6	0	-2.752872	-1.793743	-0.677386
21	1	0	-2.647282	-2.793106	-1.093824
22	6	0	-4.023272	-1.270635	-0.404086
23	1	0	-4.908542	-1.868563	-0.603447
24	6	0	-4.152232	0.017675	0.117145
25	1	0	-5.138418	0.425870	0.321013
26	6	0	-3.016340	0.796948	0.376356
27	1	0	-3.136783	1.805241	0.761214
28	6	0	1.814280	-0.573745	-2.042918
29	6	0	1.757342	1.464908	-0.983009
30	8	0	2.558699	0.514136	-1.611406
31	8	0	2.233625	2.442349	-0.482541
32	8	0	2.325207	-1.506234	-2.597326
33	6	0	-0.616247	2.355947	0.944088
34	1	0	-0.609638	2.423055	2.049694
35	8	0	-0.870201	3.331760	0.272920

Rotational constants (GHZ): 0.3746033 0.2672031 0.2547376
Standard basis: 6-31+G(d) (6D, 7F)
There are 461 symmetry adapted basis functions of A symmetry.

This journal is © The Royal Society of Chemistry 2014

```
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   461 basis functions,   784 primitive gaussians,   461 cartesian
basis functions
    79 alpha electrons       79 beta electrons
       nuclear repulsion energy      1927.9237918996 Hartrees.
 NAtoms=   35 NActive=   35 NUniq=   35 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   461 RedAO= T  NBF=   461
 NBsUse=   456 1.00D-06 NBFU=   456
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on            energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1032.18960843     A.U. after   11 cycles
            Convg  =    0.7643D-08             -V/T =  2.0093
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000003479   -0.000001517   -0.000003631
      2        6          -0.000006661   -0.000006480    0.000005253
      3        1          -0.000001446    0.000001593   -0.000002814
      4        6           0.000003214    0.000002348    0.000002421
      5        6          -0.000004714    0.000018927    0.000009628
      6        1          -0.000001966    0.000001758   -0.000002137
      7        6          -0.000002758   -0.000001820   -0.000001613
      8        6          -0.000000350    0.000008871   -0.000012686
      9        6          -0.000003320   -0.000009965    0.000023659
     10        6           0.000006832   -0.000005801   -0.000022195
     11        1          -0.000002601    0.000002986    0.000007240
     12        6           0.000001137   -0.000001015   -0.000003139
     13        1          -0.000000430   -0.000001197   -0.000003719
     14        6           0.000007947   -0.000002483   -0.000000064
     15        1           0.000001538   -0.000001906    0.000000350
     16        6           0.000000476    0.000000078   -0.000001652
     17        1           0.000003159   -0.000004042   -0.000002762
     18        6           0.000001434   -0.000003499   -0.000004573
     19        1           0.000001761   -0.000003061   -0.000004996
     20        6          -0.000003126    0.000003514   -0.000001111
     21        1          -0.000002369    0.000001064    0.000000888
     22        6          -0.000000265   -0.000000932    0.000003331
     23        1          -0.000000908    0.000001896    0.000002849
     24        6           0.000000199    0.000004085    0.000003598
     25        1           0.000000431    0.000001305    0.000004661
     26        6          -0.000000945   -0.000000891    0.000002439
     27        1           0.000000915    0.000000350    0.000004718
     28        6          -0.000007501   -0.000023502   -0.000015412
     29        6           0.000006875   -0.000015968   -0.000005756
     30        8          -0.000002806    0.000020276    0.000007439
     31        8           0.000001777    0.000005962    0.000001643
     32        8          -0.000003623    0.000009086    0.000002491
     33        6          -0.000000958    0.000008350   -0.000006938
     34        1           0.000002495   -0.000004050    0.000004176
```

```
     35        8           0.000003078   -0.000004320    0.000008413
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000023659 RMS     0.000006643


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000012797 RMS     0.000002251
 Search for a local minimum.
 Step number  10 out of a maximum of  210
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6    7    8    9
10
 DE=  1.06D-07 DEPred=-2.32D-08 R=-4.56D+00
 Trust test=-4.56D+00 RLast= 3.73D-03 DXMaxT set to 5.00D-02
     Eigenvalues ---    0.00154   0.00476   0.01057   0.01117
0.01163
     Eigenvalues ---    0.01430   0.01489   0.01690   0.01806
0.01981
     Eigenvalues ---    0.02111   0.02120   0.02131   0.02132
0.02137
     Eigenvalues ---    0.02138   0.02142   0.02149   0.02158
0.02162
     Eigenvalues ---    0.02170   0.02192   0.02796   0.03851
0.03946
     Eigenvalues ---    0.04659   0.04882   0.04937   0.05294
0.05323
     Eigenvalues ---    0.05507   0.05776   0.06223   0.06606
0.08121
     Eigenvalues ---    0.09119   0.09388   0.10005   0.12414
0.15160
     Eigenvalues ---    0.15939   0.15993   0.15999   0.16000
0.16000
     Eigenvalues ---    0.16002   0.16003   0.16049   0.16619
0.20333
     Eigenvalues ---    0.20717   0.21295   0.22001   0.22005
0.22493
     Eigenvalues ---    0.22622   0.22765   0.23754   0.24512
0.24607
     Eigenvalues ---    0.24739   0.25066   0.25820   0.27494
0.28188
     Eigenvalues ---    0.28755   0.28821   0.29482   0.29874
0.31124
     Eigenvalues ---    0.32527   0.34386   0.34426   0.34532
0.35126
```

Eigenvalues --- 0.35169 0.35233 0.35244 0.35248
0.35317
Eigenvalues --- 0.35351 0.35423 0.36716 0.39963
0.42017
Eigenvalues --- 0.42120 0.43120 0.43749 0.44225
0.44877
Eigenvalues --- 0.46059 0.46179 0.46327 0.46469
0.46817
Eigenvalues --- 0.49566 0.97829 1.04929
1.059771000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    10    9    8    7
6
 RFO step:  Lambda= 0.00000000D+00.
 DIIS coeffs:      1.18742     -0.09199     -0.24413      0.09329
0.05540
 Iteration  1 RMS(Cart)=  0.00009031 RMS(Int)=  0.00000001
 Iteration  2 RMS(Cart)=  0.00000001 RMS(Int)=  0.00000001
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86394   0.00000  -0.00002  -0.00001  -0.00003
2.86391
    R2        2.65713   0.00000   0.00000   0.00000   0.00001
2.65714
    R3        2.63128   0.00000   0.00000   0.00000   0.00000
2.63128
    R4        2.06493   0.00000   0.00000   0.00000   0.00000
2.06493
    R5        2.97110   0.00000   0.00001   0.00002   0.00003
2.97113
    R6        2.86853   0.00000   0.00000   0.00000   0.00000
2.86853
    R7        2.92024   0.00000  -0.00001   0.00001   0.00000
2.92024
    R8        2.63576   0.00000   0.00000   0.00001   0.00001
2.63576
    R9        2.06742   0.00000   0.00000   0.00001   0.00000
2.06743
   R10        2.91339  -0.00001  -0.00003  -0.00001  -0.00004
2.91335
   R11        2.87189   0.00000   0.00003  -0.00001   0.00002
2.87191
   R12        2.66163   0.00000   0.00000   0.00000   0.00001
2.66163
   R13        2.63280   0.00000   0.00000   0.00000   0.00000
2.63280
   R14        2.89804  -0.00001  -0.00004  -0.00001  -0.00006
2.89798
   R15        2.63746   0.00000   0.00000   0.00001   0.00001
2.63747
   R16        2.97628   0.00001   0.00005   0.00002   0.00007
2.97635
```

This journal is © The Royal Society of Chemistry 2014

R17	2.87890	0.00000	0.00001	0.00000	0.00001
2.87891					
R18	2.06775	0.00000	0.00000	0.00000	-0.00001
2.06775					
R19	2.88565	0.00000	0.00003	-0.00001	0.00001
2.88566					
R20	2.05498	0.00000	0.00000	0.00000	0.00000
2.05498					
R21	2.64532	0.00000	0.00000	0.00000	0.00000
2.64532					
R22	2.05162	0.00000	0.00000	0.00000	0.00000
2.05162					
R23	2.64721	0.00000	0.00000	0.00000	-0.00001
2.64720					
R24	2.05338	0.00000	0.00000	0.00000	0.00000
2.05338					
R25	2.63800	0.00000	0.00000	0.00000	0.00000
2.63800					
R26	2.05335	0.00000	0.00000	0.00000	0.00000
2.05335					
R27	2.05563	0.00000	0.00000	0.00000	0.00000
2.05563					
R28	2.64714	0.00000	0.00000	0.00000	0.00000
2.64713					
R29	2.05361	0.00000	0.00000	0.00000	0.00000
2.05361					
R30	2.63754	0.00000	0.00000	0.00000	0.00000
2.63755					
R31	2.05342	0.00000	0.00000	0.00000	0.00000
2.05342					
R32	2.64879	0.00000	0.00000	0.00000	0.00000
2.64879					
R33	2.05214	0.00000	0.00000	0.00000	0.00000
2.05214					
R34	2.62110	0.00001	0.00001	0.00003	0.00003
2.62114					
R35	2.26606	-0.00001	-0.00001	0.00000	-0.00001
2.26604					
R36	2.63278	-0.00001	-0.00001	-0.00002	-0.00003
2.63275					
R37	2.26192	0.00001	0.00000	0.00001	0.00001
2.26193					
R38	2.09318	0.00000	0.00002	0.00000	0.00001
2.09319					
R39	2.28896	-0.00001	-0.00002	0.00000	-0.00002
2.28895					
A1	1.98140	0.00000	-0.00001	0.00000	-0.00001
1.98139					
A2	2.19888	0.00000	0.00001	0.00000	0.00001
2.19889					
A3	2.10253	0.00000	-0.00001	0.00001	0.00000
2.10253					

This journal is © The Royal Society of Chemistry 2014

A4	1.97326	0.00000	0.00001	0.00000	0.00002
1.97327					
A5	1.82794	0.00000	-0.00001	-0.00001	-0.00002
1.82792					
A6	1.87826	0.00000	0.00002	0.00001	0.00003
1.87829					
A7	1.92734	0.00000	0.00000	-0.00001	-0.00001
1.92733					
A8	1.96620	0.00000	0.00000	0.00001	0.00001
1.96620					
A9	1.88357	0.00000	-0.00002	-0.00001	-0.00002
1.88355					
A10	1.97590	0.00000	0.00001	0.00000	0.00001
1.97591					
A11	2.09412	0.00000	0.00000	-0.00001	-0.00001
2.09411					
A12	2.21313	0.00000	-0.00001	0.00001	0.00000
2.21312					
A13	1.89676	0.00000	0.00001	0.00000	0.00001
1.89676					
A14	1.91447	0.00000	0.00002	0.00001	0.00003
1.91450					
A15	1.96496	0.00000	-0.00004	0.00000	-0.00004
1.96491					
A16	1.97396	0.00000	0.00000	0.00001	0.00001
1.97397					
A17	1.88815	0.00000	-0.00001	-0.00001	-0.00002
1.88813					
A18	1.82611	0.00000	0.00001	0.00000	0.00001
1.82612					
A19	1.98887	0.00000	0.00000	0.00000	0.00000
1.98888					
A20	2.19084	0.00000	0.00001	0.00000	0.00001
2.19084					
A21	2.10341	0.00000	-0.00001	0.00000	-0.00001
2.10340					
A22	1.96953	0.00000	0.00000	0.00001	0.00001
1.96954					
A23	2.09039	0.00000	0.00001	-0.00001	0.00000
2.09039					
A24	2.22207	0.00000	-0.00001	0.00000	-0.00001
2.22206					
A25	1.86889	0.00000	0.00002	0.00003	0.00005
1.86894					
A26	1.84205	0.00000	-0.00001	-0.00001	-0.00002
1.84203					
A27	1.91889	0.00000	-0.00003	0.00001	-0.00001
1.91888					
A28	1.85009	0.00000	-0.00001	-0.00002	-0.00003
1.85006					
A29	2.02018	0.00000	0.00000	0.00000	0.00000
2.02017					

This journal is © The Royal Society of Chemistry 2014

A30	1.95322	0.00000	0.00002	-0.00001	0.00002
1.95323					
A31	1.92490	0.00000	-0.00002	-0.00001	-0.00003
1.92487					
A32	1.97953	0.00000	0.00004	0.00002	0.00005
1.97958					
A33	1.81510	0.00000	-0.00001	0.00001	0.00001
1.81510					
A34	1.89409	0.00000	-0.00002	-0.00002	-0.00004
1.89406					
A35	1.96358	0.00000	0.00000	0.00000	0.00000
1.96358					
A36	1.88690	0.00000	0.00001	0.00000	0.00001
1.88691					
A37	2.09568	0.00000	0.00000	0.00000	0.00000
2.09569					
A38	2.08627	0.00000	0.00000	0.00000	0.00000
2.08627					
A39	2.10122	0.00000	0.00000	0.00000	0.00000
2.10122					
A40	2.11670	0.00000	-0.00002	0.00000	-0.00001
2.11669					
A41	2.08676	0.00000	0.00000	0.00000	0.00000
2.08676					
A42	2.07963	0.00000	0.00002	-0.00001	0.00001
2.07964					
A43	2.08479	0.00000	0.00001	0.00000	0.00001
2.08480					
A44	2.10350	0.00000	0.00000	0.00000	0.00000
2.10349					
A45	2.09484	0.00000	0.00000	0.00000	0.00000
2.09484					
A46	2.09577	0.00000	0.00001	0.00000	0.00000
2.09578					
A47	2.09189	0.00000	-0.00001	0.00000	0.00000
2.09189					
A48	2.09547	0.00000	0.00000	0.00000	0.00000
2.09547					
A49	2.09611	0.00000	0.00000	0.00000	0.00000
2.09611					
A50	2.08597	0.00000	0.00000	0.00000	0.00001
2.08598					
A51	2.10110	0.00000	0.00000	0.00000	-0.00001
2.10110					
A52	2.09154	0.00000	0.00000	0.00000	0.00000
2.09154					
A53	2.09595	0.00000	0.00000	0.00000	0.00000
2.09595					
A54	2.09568	0.00000	0.00000	0.00000	0.00000
2.09568					
A55	2.09516	0.00000	0.00000	0.00000	0.00000
2.09516					

This journal is © The Royal Society of Chemistry 2014

A56	2.10291	0.00000	0.00000	0.00000	0.00000
2.10290					
A57	2.08510	0.00000	0.00001	0.00000	0.00001
2.08511					
A58	2.08470	0.00000	0.00000	0.00001	0.00001
2.08471					
A59	2.11341	0.00000	-0.00001	0.00001	0.00000
2.11340					
A60	2.08502	0.00000	0.00001	-0.00001	-0.00001
2.08502					
A61	1.91742	0.00000	-0.00001	-0.00001	-0.00002
1.91740					
A62	2.24216	0.00001	0.00001	0.00002	0.00003
2.24219					
A63	2.12360	0.00000	0.00000	-0.00001	0.00000
2.12359					
A64	1.91439	0.00000	0.00000	0.00000	0.00000
1.91439					
A65	2.25466	0.00000	0.00000	-0.00001	0.00000
2.25466					
A66	2.11413	0.00000	-0.00001	0.00001	0.00001
2.11414					
A67	1.94644	0.00000	0.00000	0.00000	0.00001
1.94644					
A68	2.02752	-0.00001	-0.00005	0.00000	-0.00006
2.02746					
A69	2.15232	0.00000	0.00003	0.00001	0.00004
2.15236					
A70	2.10078	0.00000	0.00003	-0.00001	0.00002
2.10080					
D1	-3.13974	0.00000	-0.00001	0.00001	0.00000
3.13974					
D2	-1.04050	0.00000	-0.00001	-0.00001	-0.00002
1.04052					
D3	0.96079	0.00000	-0.00003	-0.00002	-0.00004
0.96074					
D4	-0.02757	0.00000	-0.00003	0.00000	-0.00004
0.02760					
D5	2.07167	0.00000	-0.00003	-0.00002	-0.00005
2.07162					
D6	-2.21023	0.00000	-0.00005	-0.00002	-0.00008
2.21031					
D7	-0.02727	0.00000	0.00001	0.00001	0.00002
0.02725					
D8	3.10493	0.00000	-0.00002	-0.00001	-0.00004
3.10489					
D9	-3.14124	0.00000	0.00003	0.00002	0.00005
3.14119					
D10	-0.00905	0.00000	0.00000	0.00000	0.00000
0.00905					
D11	0.02614	0.00000	0.00004	0.00002	0.00006
0.02620					

This journal is © The Royal Society of Chemistry 2014

D12	-3.11778	0.00000	0.00003	0.00000	0.00003	-3.11775
D13	3.13644	0.00000	0.00001	0.00001	0.00002	3.13646
D14	-0.00749	0.00000	0.00001	-0.00001	0.00000	-0.00749
D15	-1.09443	0.00000	0.00000	-0.00001	-0.00002	-1.09445
D16	1.07175	0.00000	0.00002	0.00000	0.00002	1.07177
D17	3.09743	0.00000	0.00002	0.00000	0.00003	3.09746
D18	1.03512	0.00000	0.00000	-0.00002	-0.00002	1.03510
D19	-3.08189	0.00000	0.00003	-0.00001	0.00002	-3.08187
D20	-1.05621	0.00000	0.00003	0.00000	0.00003	-1.05618
D21	-3.09199	0.00000	-0.00001	-0.00002	-0.00003	-3.09202
D22	-0.92581	0.00000	0.00002	-0.00001	0.00001	-0.92581
D23	1.09987	0.00000	0.00002	-0.00001	0.00001	1.09989
D24	-0.93642	0.00000	0.00001	-0.00004	-0.00003	-0.93645
D25	2.21709	0.00000	0.00003	0.00002	0.00006	2.21715
D26	-3.12331	0.00000	-0.00002	-0.00006	-0.00008	-3.12338
D27	0.03021	0.00000	0.00001	0.00000	0.00001	0.03022
D28	1.02755	0.00000	-0.00001	-0.00005	-0.00005	1.02750
D29	-2.10212	0.00000	0.00002	0.00002	0.00003	-2.10208
D30	-0.92281	0.00000	0.00000	0.00002	0.00003	-0.92278
D31	1.04297	0.00000	0.00000	0.00000	0.00000	1.04297
D32	-3.13079	0.00000	0.00001	0.00000	0.00001	-3.13079
D33	2.22895	0.00000	0.00004	0.00005	0.00009	2.22904
D34	-2.08846	0.00000	0.00003	0.00003	0.00006	-2.08840
D35	0.02096	0.00000	0.00004	0.00002	0.00007	0.02103
D36	0.01888	0.00000	-0.00001	0.00001	0.00000	0.01888
D37	-3.11138	0.00000	-0.00001	0.00001	0.00000	-3.11138

This journal is © The Royal Society of Chemistry 2014

D38	-3.13350	0.00000	-0.00005	-0.00002	-0.00006	-3.13356
D39	0.01943	0.00000	-0.00005	-0.00002	-0.00007	0.01936
D40	-0.08382	0.00000	-0.00001	0.00002	0.00001	-0.08381
D41	-2.21232	0.00000	0.00000	0.00004	0.00004	-2.21228
D42	2.02533	0.00000	-0.00002	0.00002	0.00000	2.02533
D43	2.03663	0.00000	0.00002	0.00003	0.00004	2.03668
D44	-0.09186	0.00000	0.00003	0.00005	0.00008	-0.09179
D45	-2.13740	0.00000	0.00001	0.00003	0.00004	-2.13736
D46	-2.19557	0.00000	0.00002	0.00002	0.00004	-2.19554
D47	1.95911	0.00000	0.00003	0.00004	0.00007	1.95918
D48	-0.08642	0.00000	0.00001	0.00002	0.00003	-0.08639
D49	-2.02582	0.00000	-0.00006	-0.00001	-0.00007	-2.02589
D50	1.11233	0.00000	-0.00007	-0.00004	-0.00011	1.11222
D51	2.16107	0.00000	-0.00004	0.00000	-0.00004	2.16102
D52	-0.98397	0.00000	-0.00006	-0.00002	-0.00008	-0.98405
D53	0.05217	0.00000	-0.00005	0.00000	-0.00005	0.05211
D54	-3.09287	0.00000	-0.00006	-0.00003	-0.00009	-3.09296
D55	-0.02348	0.00000	0.00000	0.00007	0.00008	-0.02340
D56	-3.11637	0.00000	0.00002	0.00005	0.00007	-3.11630
D57	3.10685	0.00000	-0.00002	0.00002	0.00000	3.10685
D58	0.01396	0.00000	-0.00001	0.00000	-0.00001	0.01395
D59	-0.00139	0.00000	-0.00002	-0.00005	-0.00007	-0.00146
D60	3.13475	0.00000	-0.00003	-0.00004	-0.00007	3.13468
D61	-3.13034	0.00000	0.00000	0.00002	0.00002	-3.13032
D62	0.00580	0.00000	-0.00001	0.00003	0.00002	0.00582
D63	0.94730	0.00000	-0.00002	-0.00008	-0.00009	0.94721

This journal is © The Royal Society of Chemistry 2014

D64	-1.01298	0.00000	-0.00002	-0.00006	-0.00008	-1.01306
D65	3.09373	0.00000	-0.00004	-0.00003	-0.00007	3.09366
D66	-2.24744	0.00000	-0.00003	-0.00006	-0.00009	-2.24753
D67	2.07545	0.00000	-0.00003	-0.00004	-0.00007	2.07538
D68	-0.10102	0.00000	-0.00005	-0.00001	-0.00007	-0.10108
D69	3.10193	0.00000	0.00002	0.00002	0.00003	3.10197
D70	-0.02455	0.00000	0.00002	-0.00003	-0.00002	-0.02456
D71	0.01678	0.00000	0.00003	0.00000	0.00002	0.01680
D72	-3.10970	0.00000	0.00003	-0.00006	-0.00002	-3.10973
D73	-0.93658	0.00000	0.00001	-0.00001	-0.00001	-0.93658
D74	1.24164	0.00000	0.00003	-0.00001	0.00002	1.24166
D75	-2.95441	0.00000	0.00003	-0.00002	0.00000	-2.95441
D76	1.04235	0.00000	0.00003	0.00000	0.00003	1.04238
D77	-3.06262	0.00000	0.00005	0.00000	0.00005	-3.06257
D78	-0.97549	0.00000	0.00004	-0.00001	0.00004	-0.97545
D79	-3.02346	0.00000	0.00003	-0.00002	0.00001	-3.02345
D80	-0.84524	0.00000	0.00005	-0.00002	0.00003	-0.84521
D81	1.24189	0.00000	0.00005	-0.00003	0.00002	1.24191
D82	1.60795	0.00000	-0.00009	-0.00012	-0.00021	1.60775
D83	-1.45687	0.00000	-0.00009	-0.00010	-0.00019	-1.45706
D84	-0.51190	0.00000	-0.00009	-0.00017	-0.00026	-0.51216
D85	2.70646	0.00000	-0.00009	-0.00015	-0.00024	2.70622
D86	-2.63410	0.00000	-0.00009	-0.00013	-0.00023	-2.63433
D87	0.58426	0.00000	-0.00010	-0.00011	-0.00021	0.58405
D88	0.09690	0.00000	0.00004	-0.00003	0.00000	0.09690
D89	-3.04539	0.00000	0.00004	-0.00006	-0.00003	-3.04541

This journal is © The Royal Society of Chemistry 2014

D90	2.17990	0.00000	0.00001	-0.00003	-0.00002	2.17987
D91	-0.96239	0.00000	0.00001	-0.00007	-0.00006	-0.96244
D92	-2.01198	0.00000	-0.00001	-0.00006	-0.00007	-2.01205
D93	1.12892	0.00000	-0.00001	-0.00009	-0.00010	1.12882
D94	-0.01479	0.00000	0.00001	-0.00002	-0.00001	-0.01480
D95	3.13788	0.00000	0.00001	-0.00001	0.00000	3.13788
D96	3.12133	0.00000	0.00000	-0.00001	-0.00001	3.12132
D97	-0.00919	0.00000	0.00000	-0.00001	0.00000	-0.00919
D98	-3.13752	0.00000	0.00000	0.00002	0.00002	-3.13750
D99	0.01569	0.00000	-0.00002	0.00005	0.00003	0.01572
D100	0.01886	0.00000	0.00000	-0.00003	-0.00003	0.01883
D101	-3.11111	0.00000	-0.00001	0.00000	-0.00002	-3.11113
D102	0.00409	0.00000	0.00000	-0.00002	-0.00002	0.00408
D103	3.13459	0.00000	0.00000	-0.00002	-0.00002	3.13457
D104	-3.12581	0.00000	-0.00001	0.00000	-0.00001	-3.12582
D105	0.00468	0.00000	-0.00001	0.00000	-0.00001	0.00467
D106	-3.13277	0.00000	-0.00001	0.00001	0.00000	-3.13277
D107	0.01403	0.00000	0.00000	0.00002	0.00002	0.01405
D108	0.00649	0.00000	-0.00001	-0.00001	-0.00002	0.00646
D109	-3.12990	0.00000	-0.00001	0.00000	-0.00001	-3.12991
D110	3.13258	0.00000	0.00000	-0.00001	-0.00002	3.13257
D111	-0.00413	0.00000	-0.00001	-0.00001	-0.00002	-0.00415
D112	-0.00379	0.00000	0.00000	0.00000	0.00000	-0.00379
D113	-3.14050	0.00000	-0.00001	0.00000	0.00000	-3.14051
D114	-0.01238	0.00000	0.00002	-0.00001	0.00001	-0.01237
D115	3.11806	0.00000	0.00002	-0.00001	0.00001	3.11807

This journal is © The Royal Society of Chemistry 2014

```
   D116        3.13406   0.00000   0.00001   0.00000   0.00001
3.13407
   D117       -0.01868   0.00000   0.00001   0.00000   0.00001  -
0.01867
   D118        0.00915   0.00000   0.00008  -0.00002   0.00006
0.00921
   D119       -3.12927   0.00000   0.00009   0.00000   0.00009  -
3.12918
   D120       -0.06880   0.00000  -0.00007   0.00003  -0.00004  -
0.06884
   D121        3.07342   0.00000  -0.00007   0.00006  -0.00001
3.07341
         Item               Value     Threshold  Converged?
 Maximum Force            0.000013     0.000450     YES
 RMS     Force            0.000002     0.000300     YES
 Maximum Displacement     0.000469     0.001800     YES
 RMS     Displacement     0.000090     0.001200     YES
 Predicted change in Energy=-4.076590D-09
 Optimization completed.
    -- Stationary point found.
                           ----------------------------
                           !   Optimized Parameters   !
                           ! (Angstroms and Degrees)  !
 --------------------------                            ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ---------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.5155         -DE/DX =    0.0
!
 ! R2    R(1,4)                  1.4061         -DE/DX =    0.0
!
 ! R3    R(1,20)                 1.3924         -DE/DX =    0.0
!
 ! R4    R(2,3)                  1.0927         -DE/DX =    0.0
!
 ! R5    R(2,5)                  1.5722         -DE/DX =    0.0
!
 ! R6    R(2,7)                  1.518          -DE/DX =    0.0
!
 ! R7    R(4,9)                  1.5453         -DE/DX =    0.0
!
 ! R8    R(4,26)                 1.3948         -DE/DX =    0.0
!
 ! R9    R(5,6)                  1.094          -DE/DX =    0.0
!
 ! R10   R(5,10)                 1.5417         -DE/DX =    0.0
!
 ! R11   R(5,28)                 1.5197         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R12   R(7,8)                  1.4085         -DE/DX =    0.0
!
 ! R13   R(7,12)                 1.3932         -DE/DX =    0.0
!
 ! R14   R(8,9)                  1.5336         -DE/DX =    0.0
!
 ! R15   R(8,14)                 1.3957         -DE/DX =    0.0
!
 ! R16   R(9,10)                 1.575          -DE/DX =    0.0
!
 ! R17   R(9,33)                 1.5234         -DE/DX =    0.0
!
 ! R18   R(10,11)                1.0942         -DE/DX =    0.0
!
 ! R19   R(10,29)                1.527          -DE/DX =    0.0
!
 ! R20   R(12,13)                1.0875         -DE/DX =    0.0
!
 ! R21   R(12,18)                1.3998         -DE/DX =    0.0
!
 ! R22   R(14,15)                1.0857         -DE/DX =    0.0
!
 ! R23   R(14,16)                1.4008         -DE/DX =    0.0
!
 ! R24   R(16,17)                1.0866         -DE/DX =    0.0
!
 ! R25   R(16,18)                1.396          -DE/DX =    0.0
!
 ! R26   R(18,19)                1.0866         -DE/DX =    0.0
!
 ! R27   R(20,21)                1.0878         -DE/DX =    0.0
!
 ! R28   R(20,22)                1.4008         -DE/DX =    0.0
!
 ! R29   R(22,23)                1.0867         -DE/DX =    0.0
!
 ! R30   R(22,24)                1.3957         -DE/DX =    0.0
!
 ! R31   R(24,25)                1.0866         -DE/DX =    0.0
!
 ! R32   R(24,26)                1.4017         -DE/DX =    0.0
!
 ! R33   R(26,27)                1.0859         -DE/DX =    0.0
!
 ! R34   R(28,30)                1.387          -DE/DX =    0.0
!
 ! R35   R(28,32)                1.1991         -DE/DX =    0.0
!
 ! R36   R(29,30)                1.3932         -DE/DX =    0.0
!
 ! R37   R(29,31)                1.197          -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R38   R(33,34)              1.1077         -DE/DX =    0.0
!
 ! R39   R(33,35)              1.2113         -DE/DX =    0.0
!
 ! A1    A(2,1,4)             113.5257         -DE/DX =    0.0
!
 ! A2    A(2,1,20)            125.9867         -DE/DX =    0.0
!
 ! A3    A(4,1,20)            120.4663         -DE/DX =    0.0
!
 ! A4    A(1,2,3)             113.0594         -DE/DX =    0.0
!
 ! A5    A(1,2,5)             104.7333         -DE/DX =    0.0
!
 ! A6    A(1,2,7)             107.6163         -DE/DX =    0.0
!
 ! A7    A(3,2,5)             110.4283         -DE/DX =    0.0
!
 ! A8    A(3,2,7)             112.6548         -DE/DX =    0.0
!
 ! A9    A(5,2,7)             107.9207         -DE/DX =    0.0
!
 ! A10   A(1,4,9)             113.2107         -DE/DX =    0.0
!
 ! A11   A(1,4,26)            119.9841         -DE/DX =    0.0
!
 ! A12   A(9,4,26)            126.8027         -DE/DX =    0.0
!
 ! A13   A(2,5,6)             108.6761         -DE/DX =    0.0
!
 ! A14   A(2,5,10)            109.6911         -DE/DX =    0.0
!
 ! A15   A(2,5,28)            112.5836         -DE/DX =    0.0
!
 ! A16   A(6,5,10)            113.0994         -DE/DX =    0.0
!
 ! A17   A(6,5,28)            108.1828         -DE/DX =    0.0
!
 ! A18   A(10,5,28)           104.6283         -DE/DX =    0.0
!
 ! A19   A(2,7,8)             113.9541         -DE/DX =    0.0
!
 ! A20   A(2,7,12)            125.5257         -DE/DX =    0.0
!
 ! A21   A(8,7,12)            120.5166         -DE/DX =    0.0
!
 ! A22   A(7,8,9)             112.8459         -DE/DX =    0.0
!
 ! A23   A(7,8,14)            119.7704         -DE/DX =    0.0
!
 ! A24   A(9,8,14)            127.3154         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A25   A(4,9,8)              107.0796         -DE/DX =    0.0
!
 ! A26   A(4,9,10)             105.5416         -DE/DX =    0.0
!
 ! A27   A(4,9,33)             109.9442         -DE/DX =    0.0
!
 ! A28   A(8,9,10)             106.0024         -DE/DX =    0.0
!
 ! A29   A(8,9,33)             115.7476         -DE/DX =    0.0
!
 ! A30   A(10,9,33)            111.9111         -DE/DX =    0.0
!
 ! A31   A(5,10,9)             110.2887         -DE/DX =    0.0
!
 ! A32   A(5,10,11)            113.4186         -DE/DX =    0.0
!
 ! A33   A(5,10,29)            103.9973         -DE/DX =    0.0
!
 ! A34   A(9,10,11)            108.5236         -DE/DX =    0.0
!
 ! A35   A(9,10,29)            112.505          -DE/DX =    0.0
!
 ! A36   A(11,10,29)           108.1114         -DE/DX =    0.0
!
 ! A37   A(7,12,13)            120.0738         -DE/DX =    0.0
!
 ! A38   A(7,12,18)            119.5343         -DE/DX =    0.0
!
 ! A39   A(13,12,18)           120.3911         -DE/DX =    0.0
!
 ! A40   A(8,14,15)            121.2779         -DE/DX =    0.0
!
 ! A41   A(8,14,16)            119.5626         -DE/DX =    0.0
!
 ! A42   A(15,14,16)           119.1539         -DE/DX =    0.0
!
 ! A43   A(14,16,17)           119.4497         -DE/DX =    0.0
!
 ! A44   A(14,16,18)           120.5215         -DE/DX =    0.0
!
 ! A45   A(17,16,18)           120.0255         -DE/DX =    0.0
!
 ! A46   A(12,18,16)           120.0788         -DE/DX =    0.0
!
 ! A47   A(12,18,19)           119.8566         -DE/DX =    0.0
!
 ! A48   A(16,18,19)           120.0616         -DE/DX =    0.0
!
 ! A49   A(1,20,21)            120.0982         -DE/DX =    0.0
!
 ! A50   A(1,20,22)            119.5173         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A51   A(21,20,22)           120.3844         -DE/DX =    0.0
!
 ! A52   A(20,22,23)           119.8366         -DE/DX =    0.0
!
 ! A53   A(20,22,24)           120.0893         -DE/DX =    0.0
!
 ! A54   A(23,22,24)           120.0734         -DE/DX =    0.0
!
 ! A55   A(22,24,25)           120.044          -DE/DX =    0.0
!
 ! A56   A(22,24,26)           120.4878         -DE/DX =    0.0
!
 ! A57   A(25,24,26)           119.4676         -DE/DX =    0.0
!
 ! A58   A(4,26,24)            119.4446         -DE/DX =    0.0
!
 ! A59   A(4,26,27)            121.0892         -DE/DX =    0.0
!
 ! A60   A(24,26,27)           119.463          -DE/DX =    0.0
!
 ! A61   A(5,28,30)            109.8603         -DE/DX =    0.0
!
 ! A62   A(5,28,32)            128.4663         -DE/DX =    0.0
!
 ! A63   A(30,28,32)           121.6732         -DE/DX =    0.0
!
 ! A64   A(10,29,30)           109.6865         -DE/DX =    0.0
!
 ! A65   A(10,29,31)           129.1826         -DE/DX =    0.0
!
 ! A66   A(30,29,31)           121.1309         -DE/DX =    0.0
!
 ! A67   A(28,30,29)           111.5226         -DE/DX =    0.0
!
 ! A68   A(9,33,34)            116.1683         -DE/DX =    0.0
!
 ! A69   A(9,33,35)            123.3191         -DE/DX =    0.0
!
 ! A70   A(34,33,35)           120.3658         -DE/DX =    0.0
!
 ! D1    D(4,1,2,3)          -179.8936         -DE/DX =    0.0
!
 ! D2    D(4,1,2,5)           -59.6163         -DE/DX =    0.0
!
 ! D3    D(4,1,2,7)            55.0489         -DE/DX =    0.0
!
 ! D4    D(20,1,2,3)           -1.5794         -DE/DX =    0.0
!
 ! D5    D(20,1,2,5)          118.6979         -DE/DX =    0.0
!
 ! D6    D(20,1,2,7)         -126.6369         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D7    D(2,1,4,9)              -1.5624         -DE/DX =    0.0
!
 ! D8    D(2,1,4,26)            177.8991         -DE/DX =    0.0
!
 ! D9    D(20,1,4,9)           -179.9798         -DE/DX =    0.0
!
 ! D10   D(20,1,4,26)            -0.5183         -DE/DX =    0.0
!
 ! D11   D(2,1,20,21)             1.4979         -DE/DX =    0.0
!
 ! D12   D(2,1,20,22)          -178.6358         -DE/DX =    0.0
!
 ! D13   D(4,1,20,21)           179.7046         -DE/DX =    0.0
!
 ! D14   D(4,1,20,22)            -0.4291         -DE/DX =    0.0
!
 ! D15   D(1,2,5,6)             -62.7061         -DE/DX =    0.0
!
 ! D16   D(1,2,5,10)             61.4068         -DE/DX =    0.0
!
 ! D17   D(1,2,5,28)            177.4698         -DE/DX =    0.0
!
 ! D18   D(3,2,5,6)              59.3079         -DE/DX =    0.0
!
 ! D19   D(3,2,5,10)           -176.5792         -DE/DX =    0.0
!
 ! D20   D(3,2,5,28)            -60.5162         -DE/DX =    0.0
!
 ! D21   D(7,2,5,6)            -177.1579         -DE/DX =    0.0
!
 ! D22   D(7,2,5,10)             -53.045         -DE/DX =    0.0
!
 ! D23   D(7,2,5,28)              63.018         -DE/DX =    0.0
!
 ! D24   D(1,2,7,8)              -53.653         -DE/DX =    0.0
!
 ! D25   D(1,2,7,12)            127.0301         -DE/DX =    0.0
!
 ! D26   D(3,2,7,8)            -178.9524         -DE/DX =    0.0
!
 ! D27   D(3,2,7,12)              1.7307         -DE/DX =    0.0
!
 ! D28   D(5,2,7,8)               58.8745         -DE/DX =    0.0
!
 ! D29   D(5,2,7,12)           -120.4424         -DE/DX =    0.0
!
 ! D30   D(1,4,9,8)              -52.8732         -DE/DX =    0.0
!
 ! D31   D(1,4,9,10)              59.7575         -DE/DX =    0.0
!
 ! D32   D(1,4,9,33)           -179.3813         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D33   D(26,4,9,8)           127.7093         -DE/DX =    0.0
!
 ! D34   D(26,4,9,10)         -119.66           -DE/DX =    0.0
!
 ! D35   D(26,4,9,33)           1.2012         -DE/DX =    0.0
!
 ! D36   D(1,4,26,24)           1.0818         -DE/DX =    0.0
!
 ! D37   D(1,4,26,27)         -178.2687         -DE/DX =    0.0
!
 ! D38   D(9,4,26,24)         -179.5363         -DE/DX =    0.0
!
 ! D39   D(9,4,26,27)           1.1132         -DE/DX =    0.0
!
 ! D40   D(2,5,10,9)           -4.8026         -DE/DX =    0.0
!
 ! D41   D(2,5,10,11)         -126.7564         -DE/DX =    0.0
!
 ! D42   D(2,5,10,29)          116.043          -DE/DX =    0.0
!
 ! D43   D(6,5,10,9)           116.6905         -DE/DX =    0.0
!
 ! D44   D(6,5,10,11)           -5.2634         -DE/DX =    0.0
!
 ! D45   D(6,5,10,29)         -122.464          -DE/DX =    0.0
!
 ! D46   D(28,5,10,9)         -125.7972         -DE/DX =    0.0
!
 ! D47   D(28,5,10,11)         112.249          -DE/DX =    0.0
!
 ! D48   D(28,5,10,29)          -4.9516         -DE/DX =    0.0
!
 ! D49   D(2,5,28,30)         -116.0707         -DE/DX =    0.0
!
 ! D50   D(2,5,28,32)           63.7319         -DE/DX =    0.0
!
 ! D51   D(6,5,28,30)          123.8201         -DE/DX =    0.0
!
 ! D52   D(6,5,28,32)          -56.3773         -DE/DX =    0.0
!
 ! D53   D(10,5,28,30)           2.9889         -DE/DX =    0.0
!
 ! D54   D(10,5,28,32)        -177.2085         -DE/DX =    0.0
!
 ! D55   D(2,7,8,9)             -1.3453         -DE/DX =    0.0
!
 ! D56   D(2,7,8,14)          -178.555          -DE/DX =    0.0
!
 ! D57   D(12,7,8,9)           178.0094         -DE/DX =    0.0
!
 ! D58   D(12,7,8,14)            0.7997         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D59   D(2,7,12,13)           -0.0798         -DE/DX =    0.0
!
 ! D60   D(2,7,12,18)          179.6077         -DE/DX =    0.0
!
 ! D61   D(8,7,12,13)         -179.3552         -DE/DX =    0.0
!
 ! D62   D(8,7,12,18)            0.3323         -DE/DX =    0.0
!
 ! D63   D(7,8,9,4)             54.2766         -DE/DX =    0.0
!
 ! D64   D(7,8,9,10)           -58.0396         -DE/DX =    0.0
!
 ! D65   D(7,8,9,33)           177.2576         -DE/DX =    0.0
!
 ! D66   D(14,8,9,4)          -128.7691         -DE/DX =    0.0
!
 ! D67   D(14,8,9,10)          118.9148         -DE/DX =    0.0
!
 ! D68   D(14,8,9,33)           -5.788          -DE/DX =    0.0
!
 ! D69   D(7,8,14,15)          177.7277         -DE/DX =    0.0
!
 ! D70   D(7,8,14,16)           -1.4065         -DE/DX =    0.0
!
 ! D71   D(9,8,14,15)            0.9613         -DE/DX =    0.0
!
 ! D72   D(9,8,14,16)         -178.1728         -DE/DX =    0.0
!
 ! D73   D(4,9,10,5)           -53.6618         -DE/DX =    0.0
!
 ! D74   D(4,9,10,11)           71.1409         -DE/DX =    0.0
!
 ! D75   D(4,9,10,29)         -169.2754         -DE/DX =    0.0
!
 ! D76   D(8,9,10,5)            59.7224         -DE/DX =    0.0
!
 ! D77   D(8,9,10,11)         -175.4749         -DE/DX =    0.0
!
 ! D78   D(8,9,10,29)           -55.8912         -DE/DX =    0.0
!
 ! D79   D(33,9,10,5)         -173.2313         -DE/DX =    0.0
!
 ! D80   D(33,9,10,11)          -48.4286         -DE/DX =    0.0
!
 ! D81   D(33,9,10,29)           71.1551         -DE/DX =    0.0
!
 ! D82   D(4,9,33,34)            92.129          -DE/DX =    0.0
!
 ! D83   D(4,9,33,35)           -83.4723         -DE/DX =    0.0
!
 ! D84   D(8,9,33,34)           -29.3299         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D85   D(8,9,33,35)          155.0688         -DE/DX =    0.0
!
 ! D86   D(10,9,33,34)        -150.9231         -DE/DX =    0.0
!
 ! D87   D(10,9,33,35)          33.4757         -DE/DX =    0.0
!
 ! D88   D(5,10,29,30)           5.5518         -DE/DX =    0.0
!
 ! D89   D(5,10,29,31)        -174.4877         -DE/DX =    0.0
!
 ! D90   D(9,10,29,30)         124.8989         -DE/DX =    0.0
!
 ! D91   D(9,10,29,31)         -55.1406         -DE/DX =    0.0
!
 ! D92   D(11,10,29,30)       -115.2782         -DE/DX =    0.0
!
 ! D93   D(11,10,29,31)         64.6823         -DE/DX =    0.0
!
 ! D94   D(7,12,18,16)          -0.8474         -DE/DX =    0.0
!
 ! D95   D(7,12,18,19)         179.7873         -DE/DX =    0.0
!
 ! D96   D(13,12,18,16)        178.8391         -DE/DX =    0.0
!
 ! D97   D(13,12,18,19)         -0.5263         -DE/DX =    0.0
!
 ! D98   D(8,14,16,17)        -179.7669         -DE/DX =    0.0
!
 ! D99   D(8,14,16,18)           0.899          -DE/DX =    0.0
!
 ! D100  D(15,14,16,17)          1.0805         -DE/DX =    0.0
!
 ! D101  D(15,14,16,18)       -178.2536         -DE/DX =    0.0
!
 ! D102  D(14,16,18,12)          0.2346         -DE/DX =    0.0
!
 ! D103  D(14,16,18,19)        179.5986         -DE/DX =    0.0
!
 ! D104  D(17,16,18,12)       -179.0957         -DE/DX =    0.0
!
 ! D105  D(17,16,18,19)          0.2683         -DE/DX =    0.0
!
 ! D106  D(1,20,22,23)        -179.4943         -DE/DX =    0.0
!
 ! D107  D(1,20,22,24)           0.804          -DE/DX =    0.0
!
 ! D108  D(21,20,22,23)          0.3716         -DE/DX =    0.0
!
 ! D109  D(21,20,22,24)       -179.33           -DE/DX =    0.0
!
 ! D110  D(20,22,24,25)        179.4838         -DE/DX =    0.0
!
```

```
 ! D111  D(20,22,24,26)         -0.2366         -DE/DX =    0.0
!
 ! D112  D(23,22,24,25)         -0.2171         -DE/DX =    0.0
!
 ! D113  D(23,22,24,26)       -179.9376         -DE/DX =    0.0
!
 ! D114  D(22,24,26,4)          -0.7095         -DE/DX =    0.0
!
 ! D115  D(22,24,26,27)        178.6517         -DE/DX =    0.0
!
 ! D116  D(25,24,26,4)         179.5685         -DE/DX =    0.0
!
 ! D117  D(25,24,26,27)         -1.0704         -DE/DX =    0.0
!
 ! D118  D(5,28,30,29)           0.5244         -DE/DX =    0.0
!
 ! D119  D(32,28,30,29)       -179.294          -DE/DX =    0.0
!
 ! D120  D(10,29,30,28)         -3.9421         -DE/DX =    0.0
!
 ! D121  D(31,29,30,28)        176.0937         -DE/DX =    0.0
!
 ---------------------------------------------------------------------
-----------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.620118   -1.034121   -0.392713
      2          6           0       -0.184794   -1.436219   -0.666578
      3          1           0       -0.093717   -2.444951   -1.076684
      4          6           0       -1.748858    0.263548    0.133190
      5          6           0        0.337569   -0.373936   -1.701290
      6          1           0       -0.252488   -0.458820   -2.618644
      7          6           0        0.596603   -1.256313    0.622321
      8          6           0        0.479376    0.028435    1.187540
      9          6           0       -0.391882    0.970943    0.348228
     10          6           0        0.281569    1.033327   -1.074141
     11          1           0       -0.262492    1.760242   -1.684780
     12          6           0        1.386641   -2.228237    1.232450
     13          1           0        1.480395   -3.214563    0.784209
     14          6           0        1.172973    0.336096    2.358952
     15          1           0        1.129332    1.329146    2.795563
     16          6           0        1.956180   -0.647277    2.976948
     17          1           0        2.492360   -0.406866    3.890957
     18          6           0        2.061789   -1.923022    2.420131
     19          1           0        2.676597   -2.678159    2.902263
```

20	6	0	-2.749307	-1.808326	-0.646385
21	1	0	-2.642992	-2.809695	-1.057787
22	6	0	-4.019561	-1.288977	-0.365343
23	1	0	-4.903929	-1.891819	-0.553591
24	6	0	-4.149589	0.001858	0.149337
25	1	0	-5.135740	0.407086	0.359202
26	6	0	-3.014876	0.787458	0.394218
27	1	0	-3.136350	1.797506	0.774116
28	6	0	1.800786	-0.577178	-2.058079
29	6	0	1.744153	1.467492	-1.009806
30	8	0	2.544190	0.516391	-1.639388
31	8	0	2.220494	2.449901	-0.519219
32	8	0	2.310958	-1.510783	-2.611302
33	6	0	-0.616727	2.359946	0.932189
34	1	0	-0.600989	2.433663	2.037282
35	8	0	-0.880562	3.330662	0.257451

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.515533	0.000000			
3	H	2.188186	1.092713	0.000000		
4	C	1.406092	2.444409	3.396948	0.000000	
5	C	2.445558	1.572239	2.205730	2.850417	0.000000
6	H	2.675098	2.184136	2.519438	3.214580	1.094034
7	C	2.448166	1.517962	2.185411	2.837326	2.498971
8	C	2.834448	2.454401	3.401879	2.476279	2.920162
9	C	2.465327	2.620524	3.713167	1.545326	2.557601
10	C	2.890518	2.546027	3.498466	2.484520	1.541701
11	H	3.364677	3.355613	4.252284	2.784670	2.216995
12	C	3.620451	2.589017	2.751458	4.153158	3.625716
13	H	3.968961	2.835515	2.555983	4.790528	3.943718
14	C	4.153374	3.760115	4.598078	3.673742	4.205664
15	H	4.828003	4.621752	5.543821	4.062968	4.873301
16	C	4.928911	4.299009	4.885247	4.758557	4.957875
17	H	5.971244	5.384965	5.959785	5.705980	5.993116
18	C	4.717909	3.848621	4.140812	4.953001	4.728500
19	H	5.658753	4.739894	4.853971	5.992166	5.654484
20	C	1.392412	2.591448	2.764527	2.429259	3.563580
21	H	2.154358	2.842925	2.575306	3.415074	3.902661
22	C	2.413095	3.849398	4.153858	2.795525	4.648293
23	H	3.397785	4.742423	4.870085	3.882235	5.576243
24	C	2.786628	4.295740	4.892862	2.415005	4.868329
25	H	3.873249	5.381623	5.968072	3.397448	5.900232
26	C	2.425440	3.752251	4.598390	1.394782	4.120543
27	H	3.417391	4.609149	5.539090	2.165397	4.786534
28	C	3.832077	2.572304	2.835639	4.255402	1.519740
29	C	4.237593	3.502881	4.323130	3.867434	2.418158
30	O	4.615165	3.493766	4.005589	4.651476	2.380272
31	O	5.186976	4.572642	5.442970	4.578377	3.593989
32	O	4.539019	3.164851	3.001697	5.211774	2.452510
33	C	3.779133	4.141677	5.234132	2.512967	3.914077

This journal is © The Royal Society of Chemistry 2014

34	H	4.355345	4.739205	5.809904	3.106858	4.768692
35	O	4.474482	4.905209	5.979694	3.190073	4.364007
		6	7	8	9	10
6	H	0.000000				
7	C	3.443952	0.000000			
8	C	3.906414	1.408471	0.000000		
9	C	3.296358	2.452122	1.533577	0.000000	
10	C	2.212964	2.866998	2.482767	1.574979	0.000000
11	H	2.407580	3.893632	3.435076	2.184686	1.094207
12	C	4.544062	1.393217	2.432635	3.765601	4.144797
13	H	4.709183	2.154539	3.417858	4.605862	4.789072
14	C	5.238348	2.425666	1.395686	2.625798	3.614811
15	H	5.866846	3.419266	2.167956	2.903765	3.972508
16	C	6.018669	2.786331	2.416509	3.878428	4.694685
17	H	7.064828	3.872910	3.398538	4.771598	5.622628
18	C	5.734894	2.413169	2.798481	4.322999	4.911121
19	H	6.632150	3.397963	3.885062	5.408753	5.943321
20	C	3.456165	3.620698	4.142627	3.777703	4.176622
21	H	3.698297	3.966200	4.779713	4.619264	4.829301
22	C	4.467366	4.720754	4.938365	4.333182	4.939150
23	H	5.287138	5.660609	5.974854	5.419156	5.976357
24	C	4.802222	4.932854	4.744037	3.885749	4.711261
25	H	5.784765	5.974604	5.688501	4.777263	5.638607
26	C	4.273328	4.155937	3.662686	2.629805	3.617053
27	H	4.991842	4.825328	4.046480	2.897704	3.960075
28	C	2.131707	3.015928	3.556252	3.604828	2.422783
29	C	3.207119	3.376363	2.915283	2.579431	1.527020
30	O	3.119517	3.471441	3.534555	3.574599	2.388762
31	O	4.357050	4.204303	3.436280	3.124787	2.464559
32	O	2.770908	3.668799	4.489441	4.714141	3.599135
33	C	4.548244	3.826946	2.588936	1.523448	2.567530
34	H	5.492318	4.129439	2.770266	2.244144	3.524316
35	O	4.798601	4.832752	3.690420	2.411498	2.898523
		11	12	13	14	15
11	H	0.000000				
12	C	5.209399	0.000000			
13	H	5.820846	1.087451	0.000000		
14	C	4.521119	2.808997	3.896345	0.000000	
15	H	4.711315	3.894163	4.981374	1.085671	0.000000
16	C	5.696522	2.422206	3.409609	1.400841	2.150076
17	H	6.585925	3.407002	4.308030	2.154023	2.464036
18	C	5.984898	1.399845	2.163871	2.428446	3.403972
19	H	7.026992	2.157473	2.490940	3.412009	4.296965
20	C	4.471822	4.562063	4.681291	5.386546	6.060905
21	H	5.190783	4.671320	4.534224	6.010965	6.797701
22	C	5.015398	5.715083	5.939601	6.084821	6.584602
23	H	6.013325	6.547854	6.655746	7.097553	7.615228
24	C	4.643858	6.065995	6.514993	5.772676	6.052372
25	H	5.455038	7.088649	7.554483	6.618451	6.785070
26	C	3.583874	5.400963	6.031229	4.647793	4.820201
27	H	3.782408	6.072407	6.814343	4.818474	4.743590
28	C	3.140064	3.704739	3.890636	4.553941	5.257639

This journal is © The Royal Society of Chemistry 2014

29	C	2.137269	4.337504	5.020926	3.599282	3.857199
30	O	3.070292	4.137675	4.574440	4.230776	4.725589
31	O	2.828318	5.064448	5.859422	3.721470	3.665312
32	O	4.263882	4.017901	3.888727	5.423043	6.220581
33	C	2.708071	5.015482	5.957765	3.055265	2.753803
34	H	3.797607	5.131446	6.148562	2.765900	2.188369
35	O	2.573031	6.082120	6.977934	4.195323	3.806278

		16	17	18	19	20
16	C	0.000000				
17	H	1.086600	0.000000			
18	C	1.395967	2.155795	0.000000		
19	H	2.156168	2.483995	1.086588	0.000000	
20	C	6.051296	7.072951	5.706428	6.541403	0.000000
21	H	6.489031	7.525656	5.917522	6.633048	1.087794
22	C	6.876929	7.829388	6.718905	7.579288	1.400804
23	H	7.815029	8.755809	7.573983	8.368132	2.158235
24	C	6.759968	7.634283	6.887879	7.833129	2.422958
25	H	7.632797	8.445337	7.840998	8.776018	3.407978
26	C	5.782763	6.631986	6.101110	7.119947	2.809176
27	H	6.063274	6.801201	6.600934	7.638778	3.894823
28	C	5.037912	5.991520	4.683351	5.457669	4.920564
29	C	4.517899	5.300048	4.833316	5.775825	5.572634
30	O	4.796920	5.607121	4.760582	5.554212	5.866130
31	O	4.678201	5.261624	5.271378	6.181551	6.545808
32	O	5.665690	6.597796	5.054438	5.647642	5.436517
33	C	4.454692	5.106465	5.266140	6.333220	4.941081
34	H	4.112697	4.590592	5.120319	6.133636	5.460019
35	O	5.591669	6.208711	6.398110	7.466883	5.542411

		21	22	23	24	25
21	H	0.000000				
22	C	2.164949	0.000000			
23	H	2.491695	1.086722	0.000000		
24	C	3.410544	1.395727	2.156189	0.000000	
25	H	4.309214	2.155794	2.484329	1.086622	0.000000
26	C	3.896938	2.428560	3.412535	1.401681	2.154988
27	H	4.982527	3.406582	4.300961	2.154381	2.470422
28	C	5.072660	6.103150	6.996068	6.372984	7.411303
29	C	6.127290	6.421359	7.462580	6.182871	7.094475
30	O	6.189344	6.925704	7.902716	6.947731	7.936475
31	O	7.183795	7.276069	8.343209	6.856956	7.684979
32	O	5.351841	6.720788	7.512253	7.186645	8.243508
33	C	5.898385	5.155337	6.218131	4.319091	4.956153
34	H	6.421996	5.596185	6.628553	4.697933	5.242798
35	O	6.522269	5.619808	6.642257	4.666815	5.163738

		26	27	28	29	30
26	C	0.000000				
27	H	1.085945	0.000000			
28	C	5.573741	6.167314	0.000000		
29	C	5.008202	5.206784	2.298425	0.000000	
30	O	5.925559	6.303554	1.387028	1.393207	0.000000
31	O	5.568410	5.549245	3.421616	1.196956	2.257879
32	O	6.532959	7.216577	1.199145	3.428728	2.260188

This journal is © The Royal Society of Chemistry 2014

33	C	2.917747	2.586469	4.838674	3.184584	4.472483
34	H	3.352089	2.903160	5.621892	3.964584	5.204420
35	O	3.322933	2.775984	5.274706	3.459259	4.821519

		31	32	33	34	35
31	O	0.000000				
32	O	4.480180	0.000000			
33	C	3.188182	6.009177	0.000000		
34	H	3.807457	6.756287	1.107661	0.000000	
35	O	3.315948	6.469554	1.211268	2.012602	0.000000

Stoichiometry C19H12O4
Framework group C1[X(C19H12O4)]
Deg. of freedom 99
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.622627	-1.025893	-0.409501
2	6	0	-0.186729	-1.432502	-0.673520
3	1	0	-0.096418	-2.439170	-1.088835
4	6	0	-1.750366	0.269180	0.123005
5	6	0	0.348941	-0.366359	-1.697401
6	1	0	-0.233611	-0.443285	-2.620236
7	6	0	0.584383	-1.263573	0.623036
8	6	0	0.467765	0.018297	1.194877
9	6	0	-0.392298	0.969476	0.353802
10	6	0	0.293538	1.037394	-1.062382
11	1	0	-0.242209	1.770233	-1.673294
12	6	0	1.365063	-2.242463	1.234073
13	1	0	1.458470	-3.226511	0.780781
14	6	0	1.152626	0.316048	2.373965
15	1	0	1.109456	1.306674	2.816095
16	6	0	1.926359	-0.674308	2.992742
17	1	0	2.455724	-0.441608	3.912701
18	6	0	2.031324	-1.947176	2.429258
19	1	0	2.638793	-2.707777	2.912104
20	6	0	-2.752872	-1.793743	-0.677386
21	1	0	-2.647282	-2.793106	-1.093824
22	6	0	-4.023272	-1.270635	-0.404086
23	1	0	-4.908542	-1.868563	-0.603447
24	6	0	-4.152232	0.017675	0.117145
25	1	0	-5.138418	0.425870	0.321013
26	6	0	-3.016340	0.796948	0.376356
27	1	0	-3.136783	1.805241	0.761214
28	6	0	1.814280	-0.573745	-2.042918
29	6	0	1.757342	1.464908	-0.983009
30	8	0	2.558699	0.514136	-1.611406
31	8	0	2.233625	2.442349	-0.482541
32	8	0	2.325207	-1.506234	-2.597326

```
    33          6           0        -0.616247    2.355947    0.944088
    34          1           0        -0.609638    2.423055    2.049694
    35          8           0        -0.870201    3.331760    0.272920
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3746033      0.2672031
0.2547376


**********************************************************************

            Population analysis using the SCF density.

**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.24026 -19.18481 -19.18088 -19.18028 -
10.35349
 Alpha  occ. eigenvalues --  -10.35345 -10.30729 -10.25823 -10.25043 -
10.24956
 Alpha  occ. eigenvalues --  -10.24310 -10.23271 -10.22908 -10.22726 -
10.22514
 Alpha  occ. eigenvalues --  -10.22065 -10.22001 -10.21961 -10.21813 -
10.21746
 Alpha  occ. eigenvalues --  -10.21717 -10.21577 -10.21520  -1.15730
-1.09210
 Alpha  occ. eigenvalues --   -1.07947  -1.05318  -0.93435  -0.87930
-0.85993
 Alpha  occ. eigenvalues --   -0.82800  -0.80202  -0.77397  -0.76778
-0.75543
 Alpha  occ. eigenvalues --   -0.70992  -0.69199  -0.66602  -0.64925
-0.62811
 Alpha  occ. eigenvalues --   -0.62742  -0.60283  -0.58279  -0.57004
-0.55058
 Alpha  occ. eigenvalues --   -0.54171  -0.52808  -0.50320  -0.49911
-0.48992
 Alpha  occ. eigenvalues --   -0.48603  -0.47862  -0.47306  -0.47021
-0.46261
 Alpha  occ. eigenvalues --   -0.45772  -0.45261  -0.44953  -0.44349
-0.43514
 Alpha  occ. eigenvalues --   -0.43352  -0.41544  -0.40763  -0.40236
-0.40026
 Alpha  occ. eigenvalues --   -0.38336  -0.37713  -0.37081  -0.36876
-0.36275
 Alpha  occ. eigenvalues --   -0.35395  -0.34716  -0.32352  -0.29720
-0.28413
 Alpha  occ. eigenvalues --   -0.27999  -0.27744  -0.27489  -0.26160
 Alpha virt. eigenvalues --   -0.06814  -0.04861  -0.04501  -0.04142
-0.03445
 Alpha virt. eigenvalues --   -0.02169  -0.01993  -0.00795   0.00087
0.00388
 Alpha virt. eigenvalues --    0.00688   0.01936   0.02268   0.03365
0.03582
 Alpha virt. eigenvalues --    0.03799   0.04219   0.04585   0.05357
0.06101
 Alpha virt. eigenvalues --    0.06485   0.06539   0.07237   0.07844
0.07958
 Alpha virt. eigenvalues --    0.08373   0.09369   0.09646   0.09653
0.10141
 Alpha virt. eigenvalues --    0.10369   0.11109   0.11315   0.11961
0.12245
 Alpha virt. eigenvalues --    0.12423   0.12887   0.13043   0.13195
0.13421
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.13717   0.14115   0.14575   0.14970
0.15196
 Alpha virt. eigenvalues --    0.15390   0.15538   0.15713   0.16166
0.16414
 Alpha virt. eigenvalues --    0.16793   0.17148   0.17827   0.18067
0.18269
 Alpha virt. eigenvalues --    0.18690   0.18900   0.19532   0.19647
0.19838
 Alpha virt. eigenvalues --    0.20098   0.20301   0.20667   0.20797
0.21030
 Alpha virt. eigenvalues --    0.21438   0.21967   0.22053   0.22400
0.22549
 Alpha virt. eigenvalues --    0.22941   0.23544   0.23672   0.23752
0.24446
 Alpha virt. eigenvalues --    0.24607   0.24875   0.25204   0.25355
0.25829
 Alpha virt. eigenvalues --    0.26014   0.26342   0.26700   0.27270
0.27847
 Alpha virt. eigenvalues --    0.28141   0.28302   0.28598   0.28867
0.29065
 Alpha virt. eigenvalues --    0.29230   0.30266   0.30757   0.30833
0.31305
 Alpha virt. eigenvalues --    0.31792   0.31966   0.32234   0.32445
0.32992
 Alpha virt. eigenvalues --    0.33245   0.33673   0.34143   0.34737
0.35396
 Alpha virt. eigenvalues --    0.35565   0.35840   0.36355   0.36593
0.37181
 Alpha virt. eigenvalues --    0.37855   0.38121   0.38817   0.39234
0.40083
 Alpha virt. eigenvalues --    0.40759   0.40885   0.41358   0.41492
0.42144
 Alpha virt. eigenvalues --    0.42412   0.42990   0.44283   0.45033
0.45719
 Alpha virt. eigenvalues --    0.46877   0.48005   0.48792   0.51524
0.52701
 Alpha virt. eigenvalues --    0.56162   0.56623   0.58102   0.59253
0.61826
 Alpha virt. eigenvalues --    0.65191   0.66868   0.68068   0.68631
0.69167
 Alpha virt. eigenvalues --    0.70317   0.70547   0.70956   0.71267
0.72236
 Alpha virt. eigenvalues --    0.72633   0.72994   0.73489   0.74347
0.75148
 Alpha virt. eigenvalues --    0.75650   0.76423   0.76799   0.77379
0.78148
 Alpha virt. eigenvalues --    0.78951   0.79824   0.80215   0.80806
0.81218
 Alpha virt. eigenvalues --    0.81586   0.83020   0.83468   0.84147
0.84603
 Alpha virt. eigenvalues --    0.85342   0.85934   0.86824   0.88421
0.88817
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.89661   0.90603   0.91740   0.92050
0.93123
 Alpha virt. eigenvalues --    0.94154   0.94483   0.94881   0.96245
0.97454
 Alpha virt. eigenvalues --    0.98411   0.98977   0.99405   1.00303
1.01553
 Alpha virt. eigenvalues --    1.02595   1.02840   1.04476   1.05353
1.05976
 Alpha virt. eigenvalues --    1.06687   1.08814   1.10932   1.11827
1.13000
 Alpha virt. eigenvalues --    1.14699   1.15735   1.16452   1.16637
1.16906
 Alpha virt. eigenvalues --    1.17929   1.19881   1.21397   1.21970
1.22992
 Alpha virt. eigenvalues --    1.23738   1.24805   1.25468   1.26041
1.26791
 Alpha virt. eigenvalues --    1.28940   1.29224   1.31829   1.32866
1.32990
 Alpha virt. eigenvalues --    1.35180   1.35346   1.36024   1.36939
1.37406
 Alpha virt. eigenvalues --    1.37546   1.38485   1.39508   1.39711
1.40930
 Alpha virt. eigenvalues --    1.41552   1.41890   1.43011   1.43333
1.45042
 Alpha virt. eigenvalues --    1.45511   1.45725   1.48090   1.48687
1.49230
 Alpha virt. eigenvalues --    1.50193   1.50840   1.52382   1.53172
1.56670
 Alpha virt. eigenvalues --    1.57142   1.58617   1.60787   1.61968
1.63879
 Alpha virt. eigenvalues --    1.67064   1.68441   1.70763   1.71956
1.72433
 Alpha virt. eigenvalues --    1.73720   1.76163   1.76387   1.77464
1.77981
 Alpha virt. eigenvalues --    1.80538   1.80686   1.81604   1.82628
1.83365
 Alpha virt. eigenvalues --    1.83376   1.85233   1.86437   1.86468
1.87043
 Alpha virt. eigenvalues --    1.87890   1.89206   1.89993   1.90868
1.92612
 Alpha virt. eigenvalues --    1.93606   1.94092   1.95505   1.96501
1.97364
 Alpha virt. eigenvalues --    1.98190   1.99118   2.00273   2.01709
2.02101
 Alpha virt. eigenvalues --    2.02828   2.03852   2.05187   2.06328
2.07401
 Alpha virt. eigenvalues --    2.08463   2.09691   2.12607   2.13614
2.13779
 Alpha virt. eigenvalues --    2.15936   2.17380   2.17666   2.18732
2.20247
 Alpha virt. eigenvalues --    2.20507   2.24372   2.25902   2.26539
2.27459
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    2.28389   2.29006   2.31100   2.32131
2.33712
 Alpha virt. eigenvalues --    2.36001   2.36930   2.38093   2.40230
2.42389
 Alpha virt. eigenvalues --    2.43530   2.44896   2.48753   2.50689
2.52400
 Alpha virt. eigenvalues --    2.54185   2.57122   2.57719   2.59467
2.59778
 Alpha virt. eigenvalues --    2.62827   2.63302   2.65378   2.68323
2.68723
 Alpha virt. eigenvalues --    2.69763   2.71477   2.72515   2.74094
2.75399
 Alpha virt. eigenvalues --    2.75979   2.78986   2.79756   2.80271
2.82447
 Alpha virt. eigenvalues --    2.83739   2.84543   2.85497   2.88292
2.91279
 Alpha virt. eigenvalues --    2.92280   2.94658   2.99331   3.04402
3.08034
 Alpha virt. eigenvalues --    3.10425   3.13913   3.16667   3.23131
3.24023
 Alpha virt. eigenvalues --    3.26908   3.32758   3.40035   3.40893
4.23560
 Alpha virt. eigenvalues --    4.25203   4.27394   4.31016   4.31763
4.33766
 Alpha virt. eigenvalues --    4.36128   4.38906   4.41164   4.42946
4.45183
 Alpha virt. eigenvalues --    4.49094   4.49814   4.52481   4.56525
4.61432
 Alpha virt. eigenvalues --    4.66716   4.74094   4.75077   4.79935
4.84604
 Alpha virt. eigenvalues --    5.13846   5.38849
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   15.019446  -3.812834  -0.048824  -0.040405  -0.808617
0.031003
     2  C   -3.812834  21.352485   0.242848  -7.142783  -0.999361  -
0.023082
     3  H   -0.048824   0.242848   0.527898   0.002530  -0.004151  -
0.002777
     4  C   -0.040405  -7.142783   0.002530  27.629049   1.736622
0.016557
     5  C   -0.808617  -0.999361  -0.004151   1.736622  11.946491
0.355991
     6  H    0.031003  -0.023082  -0.002777   0.016557   0.355991
0.478851
     7  C    0.943974  -5.521490  -0.047720  -0.126879   0.179504
0.036053
     8  C    3.387490  -6.675981  -0.003319  -1.310315   0.444900
0.011702
     9  C   -2.344920   5.434467  -0.008448  -2.829241  -1.667220  -
0.022129
```

This journal is © The Royal Society of Chemistry 2014

10	C	1.666014	-1.888176	0.031424	-0.206653	-4.045784	-0.041757
11	H	-0.052454	-0.012445	-0.000102	0.078239	-0.028195	-0.003983
12	C	-0.930646	2.479949	0.019481	-0.056269	0.111245	0.011581
13	H	-0.013775	-0.032129	0.003226	-0.003176	-0.014759	-0.000006
14	C	-2.344006	1.539680	-0.001124	2.009250	0.449823	0.000249
15	H	-0.000458	0.007902	0.000002	-0.015083	0.003451	0.000000
16	C	-0.402653	0.173792	0.003209	-0.104949	0.229404	-0.000266
17	H	0.001975	0.002988	0.000000	-0.004354	0.000742	0.000000
18	C	-0.153992	-0.328555	0.009185	0.042957	-0.055765	0.001695
19	H	-0.003723	-0.018953	-0.000004	0.002548	0.000054	0.000000
20	C	-1.508854	-0.369095	0.051147	-2.849881	0.036019	-0.027941
21	H	-0.037463	-0.070341	0.003378	0.083006	0.008579	-0.000053
22	C	-0.835287	-0.776583	0.004236	-0.628890	-0.161129	-0.004701
23	H	0.004734	-0.012964	-0.000004	0.026490	-0.001493	0.000002
24	C	0.744462	0.965286	-0.001315	0.721460	0.242078	0.006706
25	H	-0.000352	0.001256	0.000000	0.023768	0.000928	0.000000
26	C	0.452950	0.117268	0.013477	-9.667313	-0.494646	-0.004378
27	H	0.031169	-0.008650	0.000002	-0.108756	-0.006486	-0.000001
28	C	-0.592874	0.838761	-0.016973	-0.575300	-1.065728	-0.081458
29	C	-0.366251	0.491192	-0.000940	0.100848	0.750952	0.006369
30	O	-0.011901	0.138248	-0.000384	-0.012265	-0.399389	0.005868
31	O	0.031982	-0.047859	0.000076	0.009992	-0.034223	-0.000625
32	O	0.010481	-0.091276	0.005036	0.010338	-0.031789	-0.001664
33	C	-1.604014	-0.598548	0.005222	-0.906037	-0.414281	-0.000613
34	H	-0.015730	0.039935	0.000000	-0.036226	0.015501	0.000002
35	O	-0.027188	0.034879	0.000015	-0.213330	0.095283	-0.000027

This journal is © The Royal Society of Chemistry 2014

		7	8	9	10	11	12
1	C	0.943974	3.387490	-2.344920	1.666014	-0.052454	-0.930646
2	C	-5.521490	-6.675981	5.434467	-1.888176	-0.012445	2.479949
3	H	-0.047720	-0.003319	-0.008448	0.031424	-0.000102	0.019481
4	C	-0.126879	-1.310315	-2.829241	-0.206653	0.078239	-0.056269
5	C	0.179504	0.444900	-1.667220	-4.045784	-0.028195	0.111245
6	H	0.036053	0.011702	-0.022129	-0.041757	-0.003983	0.011581
7	C	22.389796	9.827345	-5.141961	0.196324	-0.007512	-8.621542
8	C	9.827345	39.688082	-5.741538	-2.418086	0.002954	-8.444395
9	C	-5.141961	-5.741538	19.398078	-0.568179	0.004499	1.281441
10	C	0.196324	-2.418086	-0.568179	14.272991	0.341425	-0.049579
11	H	-0.007512	0.002954	0.004499	0.341425	0.437913	-0.002472
12	C	-8.621542	-8.444395	1.281441	-0.049579	-0.002472	13.450300
13	H	-0.067151	0.052047	0.024246	0.003031	0.000000	0.280919
14	C	-7.066415	-19.187499	2.288588	0.257005	0.027474	6.379646
15	H	0.041910	-0.100508	-0.049467	-0.016468	-0.000003	-0.016495
16	C	0.754619	-0.789458	-0.660351	-0.489286	0.003079	-1.018583
17	H	0.029323	0.032178	-0.019486	-0.001213	0.000000	0.004945
18	C	-1.692831	-0.378987	0.140028	0.059015	-0.000245	1.149671
19	H	0.002860	0.041782	0.000544	0.000401	0.000000	0.000450
20	C	1.411356	-0.265936	-1.244272	0.335493	-0.012789	-0.783922
21	H	0.004357	0.005777	0.003277	-0.000681	0.000000	-0.001180
22	C	0.194158	0.313160	0.008170	0.124862	-0.004260	-0.311330
23	H	-0.003679	-0.000198	0.003438	0.001272	0.000000	0.000314
24	C	-0.357067	-0.766981	-0.018815	-0.338712	0.009802	0.256980
25	H	0.000068	-0.003531	-0.013671	-0.001230	0.000001	-0.000227

26	C	0.954589	1.912727	-0.515698	-0.008278	-0.038532	-0.777704
27	H	0.007445	0.024770	-0.016355	0.015484	-0.000094	0.001044
28	C	-0.870380	-0.506264	0.997378	0.272375	0.020844	0.351417
29	C	-0.409296	-1.093531	-0.139145	-1.234010	-0.075778	0.425350
30	O	-0.165720	-0.143707	0.172402	-0.179799	0.004678	0.014866
31	O	0.048592	0.285407	-0.035218	-0.182478	-0.000716	-0.026941
32	O	0.137166	0.041196	-0.040734	-0.047135	-0.000622	-0.102510
33	C	-0.730978	-1.914257	-2.573267	0.427735	0.015888	0.602139
34	H	-0.005783	-0.155816	-0.098467	-0.015622	0.000160	0.006561
35	O	-0.009437	0.144154	0.002562	-0.238688	0.005130	-0.006513

		13	14	15	16	17	18
1	C	-0.013775	-2.344006	-0.000458	-0.402653	0.001975	-0.153992
2	C	-0.032129	1.539680	0.007902	0.173792	0.002988	-0.328555
3	H	0.003226	-0.001124	0.000002	0.003209	0.000000	0.009185
4	C	-0.003176	2.009250	-0.015083	-0.104949	-0.004354	0.042957
5	C	-0.014759	0.449823	0.003451	0.229404	0.000742	-0.055765
6	H	-0.000006	0.000249	0.000000	-0.000266	0.000000	0.001695
7	C	-0.067151	-7.066415	0.041910	0.754619	0.029323	-1.692831
8	C	0.052047	-19.187499	-0.100508	-0.789458	0.032178	-0.378987
9	C	0.024246	2.288588	-0.049467	-0.660351	-0.019486	0.140028
10	C	0.003031	0.257005	-0.016468	-0.489286	-0.001213	0.059015
11	H	0.000000	0.027474	-0.000003	0.003079	0.000000	-0.000245
12	C	0.280919	6.379646	-0.016495	-1.018583	0.004945	1.149671
13	H	0.531265	-0.017196	0.000018	0.008241	-0.000159	0.047239
14	C	-0.017196	23.463996	0.243818	-1.794912	0.020187	-0.151962
15	H	0.000018	0.243818	0.541869	0.148716	-0.004560	0.008396

This journal is © The Royal Society of Chemistry 2014

16	C	0.008241	-1.794912	0.148716	9.219440	0.285860	0.872570
17	H	-0.000159	0.020187	-0.004560	0.285860	0.523223	-0.057076
18	C	0.047239	-0.151962	0.008396	0.872570	-0.057076	6.471725
19	H	-0.004242	0.013712	-0.000166	-0.049270	-0.004142	0.306733
20	C	-0.004367	-0.625772	0.000830	-0.062571	-0.000131	-0.015596
21	H	0.000000	0.000372	0.000000	0.000015	0.000000	0.000473
22	C	-0.000341	-0.295098	0.000114	-0.012927	0.000023	-0.016749
23	H	0.000000	-0.000065	0.000000	-0.000004	0.000000	0.000005
24	C	-0.000117	0.587748	-0.000554	0.064843	-0.000033	0.005135
25	H	0.000000	0.000908	0.000000	0.000056	0.000000	-0.000008
26	C	0.000304	-2.193037	0.001976	-0.013749	0.000476	-0.032876
27	H	0.000000	-0.014284	0.000002	-0.002069	0.000000	0.000071
28	C	0.015431	0.421600	-0.001366	0.024885	-0.001056	-0.053677
29	C	-0.001042	0.421415	0.016111	0.011384	0.001848	0.074320
30	O	-0.000117	0.025214	-0.000133	0.007027	-0.000009	0.001952
31	O	-0.000002	-0.168892	-0.000875	-0.027503	-0.000055	-0.004525
32	O	-0.000257	-0.031500	0.000000	-0.001576	0.000002	-0.006411
33	C	0.002381	1.845897	0.004443	-0.016818	0.000020	0.058514
34	H	0.000000	0.103966	0.003386	0.051513	-0.000002	0.000157
35	O	-0.000001	0.018414	0.001691	0.025913	0.000000	-0.000001

		19	20	21	22	23	24
1	C	-0.003723	-1.508854	-0.037463	-0.835287	0.004734	0.744462
2	C	-0.018953	-0.369095	-0.070341	-0.776583	-0.012964	0.965286
3	H	-0.000004	0.051147	0.003378	0.004236	-0.000004	-0.001315
4	C	0.002548	-2.849881	0.083006	-0.628890	0.026490	0.721460
5	C	0.000054	0.036019	0.008579	-0.161129	-0.001493	0.242078

This journal is © The Royal Society of Chemistry 2014

```
     6  H    0.000000  -0.027941  -0.000053  -0.004701   0.000002
0.006706
     7  C    0.002860   1.411356   0.004357   0.194158  -0.003679  -
0.357067
     8  C    0.041782  -0.265936   0.005777   0.313160  -0.000198  -
0.766981
     9  C    0.000544  -1.244272   0.003277   0.008170   0.003438  -
0.018815
    10  C    0.000401   0.335493  -0.000681   0.124862   0.001272  -
0.338712
    11  H    0.000000  -0.012789   0.000000  -0.004260   0.000000
0.009802
    12  C    0.000450  -0.783922  -0.001180  -0.311330   0.000314
0.256980
    13  H   -0.004242  -0.004367   0.000000  -0.000341   0.000000  -
0.000117
    14  C    0.013712  -0.625772   0.000372  -0.295098  -0.000065
0.587748
    15  H   -0.000166   0.000830   0.000000   0.000114   0.000000  -
0.000554
    16  C   -0.049270  -0.062571   0.000015  -0.012927  -0.000004
0.064843
    17  H   -0.004142  -0.000131   0.000000   0.000023   0.000000  -
0.000033
    18  C    0.306733  -0.015596   0.000473  -0.016749   0.000005
0.005135
    19  H    0.522922   0.000361   0.000000  -0.000026   0.000000
0.000011
    20  C    0.000361   9.717431   0.282037   0.720576   0.000733  -
1.514087
    21  H    0.000000   0.282037   0.534413   0.017130  -0.004229
0.007945
    22  C   -0.000026   0.720576   0.017130   6.876272   0.307082
0.136327
    23  H    0.000000   0.000733  -0.004229   0.307082   0.524111  -
0.033602
    24  C    0.000011  -1.514087   0.007945   0.136327  -0.033602
9.920645
    25  H    0.000000   0.025216  -0.000158  -0.030184  -0.004198
0.332897
    26  C   -0.000249   2.690046  -0.024900   0.677866   0.003825  -
4.516332
    27  H    0.000000  -0.009752   0.000019   0.017275  -0.000157  -
0.021653
    28  C    0.000846  -0.213476   0.001898  -0.016787   0.000014
0.037655
    29  C   -0.000999   0.046205  -0.000521  -0.038926  -0.000065
0.083727
    30  O   -0.000010   0.012802   0.000000   0.002253   0.000000  -
0.000862
    31  O    0.000004   0.004065   0.000000   0.000770   0.000000  -
0.004210
```

This journal is © The Royal Society of Chemistry 2014

32	O	-0.000020	0.019278	0.000002	0.000334	0.000000	-0.000830
33	C	-0.000242	0.061809	0.001223	-0.013224	0.000687	-0.299261
34	H	0.000000	-0.004398	0.000000	-0.003254	0.000000	0.038804
35	O	0.000000	0.000719	0.000003	-0.002316	0.000002	0.042930

		25	26	27	28	29	30
1	C	-0.000352	0.452950	0.031169	-0.592874	-0.366251	-0.011901
2	C	0.001256	0.117268	-0.008650	0.838761	0.491192	0.138248
3	H	0.000000	0.013477	0.000002	-0.016973	-0.000940	-0.000384
4	C	0.023768	-9.667313	-0.108756	-0.575300	0.100848	-0.012265
5	C	0.000928	-0.494646	-0.006486	-1.065728	0.750952	-0.399389
6	H	0.000000	-0.004378	-0.000001	-0.081458	0.006369	0.005868
7	C	0.000068	0.954589	0.007445	-0.870380	-0.409296	-0.165720
8	C	-0.003531	1.912727	0.024770	-0.506264	-1.093531	-0.143707
9	C	-0.013671	-0.515698	-0.016355	0.997378	-0.139145	0.172402
10	C	-0.001230	-0.008278	0.015484	0.272375	-1.234010	-0.179799
11	H	0.000001	-0.038532	-0.000094	0.020844	-0.075778	0.004678
12	C	-0.000227	-0.777704	0.001044	0.351417	0.425350	0.014866
13	H	0.000000	0.000304	0.000000	0.015431	-0.001042	-0.000117
14	C	0.000908	-2.193037	-0.014284	0.421600	0.421415	0.025214
15	H	0.000000	0.001976	0.000002	-0.001366	0.016111	-0.000133
16	C	0.000056	-0.013749	-0.002069	0.024885	0.011384	0.007027
17	H	0.000000	0.000476	0.000000	-0.001056	0.001848	-0.000009
18	C	-0.000008	-0.032876	0.000071	-0.053677	0.074320	0.001952
19	H	0.000000	-0.000249	0.000000	0.000846	-0.000999	-0.000010
20	C	0.025216	2.690046	-0.009752	-0.213476	0.046205	0.012802
21	H	-0.000158	-0.024900	0.000019	0.001898	-0.000521	0.000000

This journal is © The Royal Society of Chemistry 2014

22	C	-0.030184	0.677866	0.017275	-0.016787	-0.038926
0.002253						
23	H	-0.004198	0.003825	-0.000157	0.000014	-0.000065
0.000000						
24	C	0.332897	-4.516332	-0.021653	0.037655	0.083727
0.000862						
25	H	0.522830	-0.036615	-0.004213	-0.000082	0.000004
0.000000						
26	C	-0.036615	17.716674	0.375071	-0.084764	0.034370
0.017523						
27	H	-0.004213	0.375071	0.520948	-0.000904	0.004075
0.000003						
28	C	-0.000082	-0.084764	-0.000904	6.672223	-0.876505
0.266312						
29	C	0.000004	0.034370	0.004075	-0.876505	6.775994
0.257191						
30	O	0.000000	0.017523	-0.000003	0.266312	0.257191
8.368487						
31	O	0.000000	-0.000080	-0.000030	0.043387	0.468610
0.073275						
32	O	0.000000	0.003454	0.000000	0.458034	0.026862
0.082988						
33	C	-0.001940	-0.343818	0.000291	0.171522	0.009638
0.011821						
34	H	0.000000	0.032209	-0.001544	0.002284	-0.000794
0.000092						
35	O	0.000026	-0.015147	-0.000714	0.002327	-0.048706
0.001363						

		31	32	33	34	35
1	C	0.031982	0.010481	-1.604014	-0.015730	-0.027188
2	C	-0.047859	-0.091276	-0.598548	0.039935	0.034879
3	H	0.000076	0.005036	0.005222	0.000000	0.000015
4	C	0.009992	0.010338	-0.906037	-0.036226	-0.213330
5	C	-0.034223	-0.031789	-0.414281	0.015501	0.095283
6	H	-0.000625	-0.001664	-0.000613	0.000002	-0.000027
7	C	0.048592	0.137166	-0.730978	-0.005783	-0.009437
8	C	0.285407	0.041196	-1.914257	-0.155816	0.144154
9	C	-0.035218	-0.040734	-2.573267	-0.098467	0.002562
10	C	-0.182478	-0.047135	0.427735	-0.015622	-0.238688
11	H	-0.000716	-0.000622	0.015888	0.000160	0.005130
12	C	-0.026941	-0.102510	0.602139	0.006561	-0.006513
13	H	-0.000002	-0.000257	0.002381	0.000000	-0.000001
14	C	-0.168892	-0.031500	1.845897	0.103966	0.018414
15	H	-0.000875	0.000000	0.004443	0.003386	0.001691
16	C	-0.027503	-0.001576	-0.016818	0.051513	0.025913
17	H	-0.000055	0.000002	0.000020	-0.000002	0.000000
18	C	-0.004525	-0.006411	0.058514	0.000157	-0.000001
19	H	0.000004	-0.000020	-0.000242	0.000000	0.000000
20	C	0.004065	0.019278	0.061809	-0.004398	0.000719
21	H	0.000000	0.000002	0.001223	0.000000	0.000003
22	C	0.000770	0.000334	-0.013224	-0.003254	-0.002316
23	H	0.000000	0.000000	0.000687	0.000000	0.000002

This journal is © The Royal Society of Chemistry 2014

24	C	-0.004210	-0.000830	-0.299261	0.038804	0.042930
25	H	0.000000	0.000000	-0.001940	0.000000	0.000026
26	C	-0.000080	0.003454	-0.343818	0.032209	-0.015147
27	H	-0.000030	0.000000	0.000291	-0.001544	-0.000714
28	C	0.043387	0.458034	0.171522	0.002284	0.002327
29	C	0.468610	0.026862	0.009638	-0.000794	-0.048706
30	O	-0.073275	-0.082988	0.011821	0.000092	0.001363
31	O	8.053653	0.000301	0.003566	0.000225	0.004832
32	O	0.000301	8.111203	-0.001214	-0.000003	-0.000013
33	C	0.003566	-0.001214	11.300456	0.287524	0.605750
34	H	0.000225	-0.000003	0.287524	0.621821	-0.041663
35	O	0.004832	-0.000013	0.605750	-0.041663	7.864782

Mulliken atomic charges:

		1
1	C	-0.368459
2	C	0.570170
3	H	0.213689
4	C	0.344455
5	C	-0.374551
6	H	0.252831
7	C	-0.313595
8	C	-0.315363
9	C	-0.010535
10	C	-0.033036
11	H	0.288116
12	C	0.322009
13	H	0.190490
14	C	-0.227202
15	H	0.181500
16	C	-0.437621
17	H	0.188488
18	C	-0.300583
19	H	0.188818
20	C	0.096718
21	H	0.185622
22	C	-0.248595
23	H	0.187951
24	C	-0.331009
25	H	0.188452
26	C	-0.236688
27	H	0.198000
28	C	0.358402
29	C	0.280043
30	O	-0.237534
31	O	-0.347954
32	O	-0.383149
33	C	0.001988
34	H	0.175162
35	O	-0.247033

Sum of Mulliken atomic charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

	1

This journal is © The Royal Society of Chemistry 2014

```
     1  C   -0.368459
     2  C    0.783860
     4  C    0.344455
     5  C   -0.121719
     7  C   -0.313595
     8  C   -0.315363
     9  C   -0.010535
    10  C    0.255080
    12  C    0.512499
    14  C   -0.045702
    16  C   -0.249133
    18  C   -0.111765
    20  C    0.282340
    22  C   -0.060644
    24  C   -0.142558
    26  C   -0.038688
    28  C    0.358402
    29  C    0.280043
    30  O   -0.237534
    31  O   -0.347954
    32  O   -0.383149
    33  C    0.177150
    35  O   -0.247033
 Sum of Mulliken charges with hydrogens summed into heavy atoms =
0.00000
 Electronic spatial extent (au):  <R**2>=           5291.3769
 Charge=              0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=             -4.2934    Y=             -3.0751    Z=
2.0765  Tot=              5.6746
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=           -136.1245   YY=           -141.2441   ZZ=           -
127.5166
   XY=             -0.8484   XZ=             11.7632   YZ=
-0.1433
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=             -1.1628   YY=             -6.2823   ZZ=
7.4451
   XY=             -0.8484   XZ=             11.7632   YZ=
-0.1433
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=            -68.0764  YYY=            -61.2626  ZZZ=
7.0602  XYY=             -5.5636
  XXY=            -10.9016  XXZ=             30.0909  XZZ=
13.2091  YZZ=             32.3773
  YYZ=              7.6687  XYZ=            -27.4663
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=          -3279.2564 YYYY=          -2108.1639 ZZZZ=          -
1747.9773 XXXY=             -3.5679
 XXXZ=             46.9070 YYYX=              1.8080 YYYZ=
10.3945 ZZZX=             76.2318
```

This journal is © The Royal Society of Chemistry 2014


```
 ZZZY=            -20.8120 XXYY=           -908.2136 XXZZ=           -
909.2950 YYZZ=           -611.8633
 XXYZ=             -9.5408 YYXZ=             46.9276 ZZXY=
17.1987
 N-N= 1.927923791900D+03 E-N=-6.255402187720D+03  KE=
1.022665953906D+03
 1|1|UNPC-MECHANOCHEM2|FOpt|RB3LYP|6-31+G(d)|C19H12O4|JAMES|24-Jul-
2013
 |0||# opt b3lyp/6-31+g(d) geom=connectivity||9-formylanthracene DA
pro
 duct||0,1|C,-1.6201175638,-1.0341212173,-0.3927133388|C,-
0.1847936268,
 -1.4362188016,-0.6665783087|H,-0.0937166659,-2.4449512373,-
1.076683566
 |C,-1.7488580472,0.2635483774,0.1331898596|C,0.3375688303,-
0.373936247
 3,-1.7012898884|H,-0.252487896,-0.4588200891,-
2.618643569|C,0.59660342
 17,-
1.2563131666,0.6223214325|C,0.479375638,0.0284348967,1.1875397884|
 C,-
0.3918822964,0.9709432067,0.3482275747|C,0.2815690415,1.0333265527,
 -1.0741405022|H,-0.2624923692,1.7602424954,-
1.6847796957|C,1.386641387
 ,-2.2282368219,1.2324499069|H,1.4803947852,-
3.2145630044,0.7842085679|

C,1.1729732029,0.3360962163,2.3589519308|H,1.1293316821,1.3291459968,2
 .7955632368|C,1.9561795692,-
0.6472771808,2.9769478733|H,2.4923604211,-
 0.4068662208,3.8909570742|C,2.0617885054,-
1.9230221735,2.4201306583|H,
 2.6765968085,-2.6781589287,2.9022630588|C,-2.7493074667,-
1.808325656,-
 0.6463845622|H,-2.6429924821,-2.8096952589,-1.0577867232|C,-
4.01956072
 64,-1.2889765481,-0.3653426523|H,-4.9039291099,-1.8918192977,-
0.553591
 4696|C,-4.149588875,0.0018576129,0.149336591|H,-
5.1357399832,0.4070855
 485,0.359202399|C,-3.014875519,0.787457754,0.3942180249|H,-
3.136349669
 ,1.7975059793,0.7741159076|C,1.8007856819,-0.5771783336,-
2.0580787494|
 C,1.7441532865,1.4674919717,-
1.0098060627|O,2.5441904941,0.5163912818,
 -1.6393879622|O,2.2204944979,2.4499010833,-
0.5192193262|O,2.3109575916
 ,-1.5107826214,-2.6113020625|C,-
0.6167270329,2.359945685,0.932188887|H
 ,-0.6009891437,2.4336633821,2.0372818503|O,-
0.8805623716,3.3306617644,
```

This journal is © The Royal Society of Chemistry 2014

```
 0.2574508172||Version=IA32W-G09RevA.02|State=1-A|HF=-
1032.1896084|RMSD
 =7.643e-009|RMSF=6.643e-006|Dipole=-1.6769473,-
1.2120896,0.8385014|Qua
 drupole=-0.7097397,-4.6764828,5.3862225,-0.5625909,8.802728,-
0.0039661
 |PG=C01 [X(C19H12O4)]||@


 LAWS OF PROGRAMMING DEFINITION:  A WORKING PROGRAM
                                  IS ONE THAT HAS
                                  ONLY UNOBSERVED
                                  BUGS.
 Job cpu time:  0 days  9 hours 25 minutes 25.0 seconds.
 File lengths (MBytes):  RWF=    133 Int=      0 D2E=      0 Chk=
14 Scr=      1
 Normal termination of Gaussian 09 at Wed Jul 24 23:36:07 2013.
```

This journal is © The Royal Society of Chemistry 2014

9-Cyanoanthracene

```
Entering Gaussian System, Link 0=g03
 Initial command:
 /usr/local/g03d01/g03/l1.exe /tmp/pbstmp.6522854/Gau-6980.inp -
scrdir=/tmp/pbstmp.6522854/
 Entering Link 1 = /usr/local/g03d01/g03/l1.exe PID=      6981.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2004, Gaussian, Inc.
                  All Rights Reserved.

 This is the Gaussian(R) 03 program.  It is based on the
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,
 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be
 used, copied, transmitted, or stored only in accord with that
 written license.

 The following legend is applicable only to US Government
 contracts under FAR:

                       RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is
 subject to restrictions as set forth in subparagraphs (a)
 and (c) of the Commercial Computer Software - Restricted
 Rights clause in FAR 52.227-19.

 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ----------------------------------------------------------------
 Warning -- This program may not be used in any manner that
 competes with the business of Gaussian, Inc. or will provide
 assistance to any competitor of Gaussian, Inc.  The licensee
 of this program is prohibited from giving any competitor of
 Gaussian, Inc. access to this program.  By using this program,
 the user acknowledges that Gaussian, Inc. is engaged in the
```

This journal is © The Royal Society of Chemistry 2014

```
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.
----------------------------------------------------------------


Cite this work as:
Gaussian 03, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

****************************************
Gaussian 03:  AM64L-G03RevD.01 13-Oct-2005
               18-Oct-2011
****************************************
%nprocshared=4
Will use up to    4 processors via shared memory.
%mem=450MW
%chk=cyanoanthracene.chk
---------------------------------------
# opt b3lyp/6-31+g(d) geom=connectivity
---------------------------------------
1/14=-1,18=20,26=3,38=1,57=2/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20/3(3);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99//99;
2/9=110/2;
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,74=-5/1,2,3;
```

```
 4/5=5,16=3/1;
 5/5=2,38=5/2;
 7//1,2,3,16;
 1/14=-1,18=20/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 ---------------
 cyanoanthracene
 ---------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                    -5.5547   -0.91341   0.05747
 C                    -4.19775  -0.91296   0.06152
 C                    -3.49874   0.29968   0.05585
 C                    -4.20739   1.50466   0.04603
 C                    -5.60691   1.48318   0.04199
 C                    -6.26684   0.29753   0.0476
 C                    -2.09738   0.30888   0.05998
 C                    -3.51822   2.72488   0.04029
 C                    -2.11685   2.73408   0.04442
 C                    -1.40821   1.5291    0.05424
 C                    -0.00868   1.55058   0.05828
 H                     0.54063   0.63237   0.06579
 C                     0.65125   2.73623   0.05267
 C                    -0.0609    3.94716   0.0428
 C                    -1.41784   3.94672   0.03875
 H                    -1.55498  -0.61343   0.0675
 H                    -6.08584  -1.84226   0.06182
 H                    -3.6623   -1.83931   0.06904
 H                    -6.15622   2.40139   0.03448
 H                    -7.33676   0.28482   0.04449
 H                     1.72117   2.74894   0.05579
 H                     0.47024   4.87602   0.03845
 H                    -1.9533    4.87307   0.03123
 C                    -4.29887   4.05231   0.02947
 N                    -4.8801    5.04064   0.02142


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Initialization pass.
                           ----------------------------
                           !    Initial Parameters    !
                           ! (Angstroms and Degrees)  !
 --------------------------                            ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ----------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.3569         estimate D2E/DX2
!
 ! R2    R(1,6)                  1.4049         estimate D2E/DX2
!
 ! R3    R(1,17)                 1.07           estimate D2E/DX2
!
 ! R4    R(2,3)                  1.3997         estimate D2E/DX2
!
 ! R5    R(2,18)                 1.07           estimate D2E/DX2
!
 ! R6    R(3,4)                  1.3979         estimate D2E/DX2
!
 ! R7    R(3,7)                  1.4014         estimate D2E/DX2
!
 ! R8    R(4,5)                  1.3997         estimate D2E/DX2
!
 ! R9    R(4,8)                  1.4014         estimate D2E/DX2
!
 ! R10   R(5,6)                  1.3569         estimate D2E/DX2
!
 ! R11   R(5,19)                 1.07           estimate D2E/DX2
!
 ! R12   R(6,20)                 1.07           estimate D2E/DX2
!
 ! R13   R(7,10)                 1.4014         estimate D2E/DX2
!
 ! R14   R(7,16)                 1.07           estimate D2E/DX2
!
 ! R15   R(8,9)                  1.4014         estimate D2E/DX2
!
 ! R16   R(8,24)                 1.54           estimate D2E/DX2
!
 ! R17   R(9,10)                 1.3979         estimate D2E/DX2
!
 ! R18   R(9,15)                 1.3997         estimate D2E/DX2
!
 ! R19   R(10,11)                1.3997         estimate D2E/DX2
!
 ! R20   R(11,12)                1.07           estimate D2E/DX2
!
 ! R21   R(11,13)                1.3569         estimate D2E/DX2
!
 ! R22   R(13,14)                1.4049         estimate D2E/DX2
!
 ! R23   R(13,21)                1.07           estimate D2E/DX2
!
 ! R24   R(14,15)                1.3569         estimate D2E/DX2
!
 ! R25   R(14,22)                1.07           estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R26   R(15,23)              1.07          estimate D2E/DX2
!
 ! R27   R(24,25)              1.1466        estimate D2E/DX2
!
 ! A1    A(2,1,6)             120.4412       estimate D2E/DX2
!
 ! A2    A(2,1,17)            119.7794       estimate D2E/DX2
!
 ! A3    A(6,1,17)            119.7794       estimate D2E/DX2
!
 ! A4    A(1,2,3)             119.9783       estimate D2E/DX2
!
 ! A5    A(1,2,18)            120.0109       estimate D2E/DX2
!
 ! A6    A(3,2,18)            120.0109       estimate D2E/DX2
!
 ! A7    A(2,3,4)             119.5806       estimate D2E/DX2
!
 ! A8    A(2,3,7)             120.3356       estimate D2E/DX2
!
 ! A9    A(4,3,7)             120.0839       estimate D2E/DX2
!
 ! A10   A(3,4,5)             119.5806       estimate D2E/DX2
!
 ! A11   A(3,4,8)             120.0839       estimate D2E/DX2
!
 ! A12   A(5,4,8)             120.3356       estimate D2E/DX2
!
 ! A13   A(4,5,6)             119.9783       estimate D2E/DX2
!
 ! A14   A(4,5,19)            120.0109       estimate D2E/DX2
!
 ! A15   A(6,5,19)            120.0109       estimate D2E/DX2
!
 ! A16   A(1,6,5)             120.4412       estimate D2E/DX2
!
 ! A17   A(1,6,20)            119.7794       estimate D2E/DX2
!
 ! A18   A(5,6,20)            119.7794       estimate D2E/DX2
!
 ! A19   A(3,7,10)            119.8322       estimate D2E/DX2
!
 ! A20   A(3,7,16)            120.0839       estimate D2E/DX2
!
 ! A21   A(10,7,16)           120.0839       estimate D2E/DX2
!
 ! A22   A(4,8,9)             119.8322       estimate D2E/DX2
!
 ! A23   A(4,8,24)            120.0839       estimate D2E/DX2
!
 ! A24   A(9,8,24)            120.0839       estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A25   A(8,9,10)             120.0839         estimate D2E/DX2
!
 ! A26   A(8,9,15)             120.3355         estimate D2E/DX2
!
 ! A27   A(10,9,15)            119.5806         estimate D2E/DX2
!
 ! A28   A(7,10,9)             120.0839         estimate D2E/DX2
!
 ! A29   A(7,10,11)            120.3356         estimate D2E/DX2
!
 ! A30   A(9,10,11)            119.5806         estimate D2E/DX2
!
 ! A31   A(10,11,12)           120.0109         estimate D2E/DX2
!
 ! A32   A(10,11,13)           119.9783         estimate D2E/DX2
!
 ! A33   A(12,11,13)           120.0109         estimate D2E/DX2
!
 ! A34   A(11,13,14)           120.4412         estimate D2E/DX2
!
 ! A35   A(11,13,21)           119.7794         estimate D2E/DX2
!
 ! A36   A(14,13,21)           119.7794         estimate D2E/DX2
!
 ! A37   A(13,14,15)           120.4412         estimate D2E/DX2
!
 ! A38   A(13,14,22)           119.7794         estimate D2E/DX2
!
 ! A39   A(15,14,22)           119.7794         estimate D2E/DX2
!
 ! A40   A(9,15,14)            119.9783         estimate D2E/DX2
!
 ! A41   A(9,15,23)            120.0109         estimate D2E/DX2
!
 ! A42   A(14,15,23)           120.0109         estimate D2E/DX2
!
 ! A43   L(8,24,25,9,-1)       179.9999         estimate D2E/DX2
!
 ! A44   L(8,24,25,9,-2)       180.0            estimate D2E/DX2
!
 ! D1    D(6,1,2,3)             -0.0002         estimate D2E/DX2
!
 ! D2    D(6,1,2,18)           179.9998         estimate D2E/DX2
!
 ! D3    D(17,1,2,3)           179.9999         estimate D2E/DX2
!
 ! D4    D(17,1,2,18)           -0.0001         estimate D2E/DX2
!
 ! D5    D(2,1,6,5)              0.0002         estimate D2E/DX2
!
 ! D6    D(2,1,6,20)          -179.9998         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D7    D(17,1,6,5)          -179.9999         estimate D2E/DX2
!
 ! D8    D(17,1,6,20)            0.0001         estimate D2E/DX2
!
 ! D9    D(1,2,3,4)              0.0            estimate D2E/DX2
!
 ! D10   D(1,2,3,7)           -180.0            estimate D2E/DX2
!
 ! D11   D(18,2,3,4)          -180.0            estimate D2E/DX2
!
 ! D12   D(18,2,3,7)             0.0001         estimate D2E/DX2
!
 ! D13   D(2,3,4,5)              0.0001         estimate D2E/DX2
!
 ! D14   D(2,3,4,8)           -180.0            estimate D2E/DX2
!
 ! D15   D(7,3,4,5)           -180.0            estimate D2E/DX2
!
 ! D16   D(7,3,4,8)              0.0            estimate D2E/DX2
!
 ! D17   D(2,3,7,10)          -180.0            estimate D2E/DX2
!
 ! D18   D(2,3,7,16)             0.0            estimate D2E/DX2
!
 ! D19   D(4,3,7,10)             0.0            estimate D2E/DX2
!
 ! D20   D(4,3,7,16)          -180.0            estimate D2E/DX2
!
 ! D21   D(3,4,5,6)              0.0            estimate D2E/DX2
!
 ! D22   D(3,4,5,19)           180.0            estimate D2E/DX2
!
 ! D23   D(8,4,5,6)           -180.0            estimate D2E/DX2
!
 ! D24   D(8,4,5,19)             0.0            estimate D2E/DX2
!
 ! D25   D(3,4,8,9)              0.0            estimate D2E/DX2
!
 ! D26   D(3,4,8,24)          -179.9999         estimate D2E/DX2
!
 ! D27   D(5,4,8,9)            179.9999         estimate D2E/DX2
!
 ! D28   D(5,4,8,24)             0.0            estimate D2E/DX2
!
 ! D29   D(4,5,6,1)             -0.0001         estimate D2E/DX2
!
 ! D30   D(4,5,6,20)           179.9999         estimate D2E/DX2
!
 ! D31   D(19,5,6,1)           179.9999         estimate D2E/DX2
!
 ! D32   D(19,5,6,20)           -0.0001         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D33   D(3,7,10,9)             0.0           estimate D2E/DX2
!
 ! D34   D(3,7,10,11)          180.0           estimate D2E/DX2
!
 ! D35   D(16,7,10,9)          180.0           estimate D2E/DX2
!
 ! D36   D(16,7,10,11)           0.0           estimate D2E/DX2
!
 ! D37   D(4,8,9,10)             0.0           estimate D2E/DX2
!
 ! D38   D(4,8,9,15)           180.0           estimate D2E/DX2
!
 ! D39   D(24,8,9,10)          179.9999        estimate D2E/DX2
!
 ! D40   D(24,8,9,15)           -0.0001        estimate D2E/DX2
!
 ! D41   D(8,9,10,7)             0.0           estimate D2E/DX2
!
 ! D42   D(8,9,10,11)         -180.0           estimate D2E/DX2
!
 ! D43   D(15,9,10,7)         -180.0           estimate D2E/DX2
!
 ! D44   D(15,9,10,11)           0.0           estimate D2E/DX2
!
 ! D45   D(8,9,15,14)         -180.0           estimate D2E/DX2
!
 ! D46   D(8,9,15,23)            0.0001        estimate D2E/DX2
!
 ! D47   D(10,9,15,14)           0.0           estimate D2E/DX2
!
 ! D48   D(10,9,15,23)        -179.9999        estimate D2E/DX2
!
 ! D49   D(7,10,11,12)          -0.0001        estimate D2E/DX2
!
 ! D50   D(7,10,11,13)        -180.0           estimate D2E/DX2
!
 ! D51   D(9,10,11,12)         179.9999        estimate D2E/DX2
!
 ! D52   D(9,10,11,13)           0.0001        estimate D2E/DX2
!
 ! D53   D(10,11,13,14)         -0.0002        estimate D2E/DX2
!
 ! D54   D(10,11,13,21)        180.0           estimate D2E/DX2
!
 ! D55   D(12,11,13,14)        180.0           estimate D2E/DX2
!
 ! D56   D(12,11,13,21)          0.0001        estimate D2E/DX2
!
 ! D57   D(11,13,14,15)          0.0002        estimate D2E/DX2
!
 ! D58   D(11,13,14,22)       -179.9998        estimate D2E/DX2
!
```

```
 ! D59   D(21,13,14,15)       -179.9999         estimate D2E/DX2
!
 ! D60   D(21,13,14,22)          0.0            estimate D2E/DX2
!
 ! D61   D(13,14,15,9)          -0.0001         estimate D2E/DX2
!
 ! D62   D(13,14,15,23)        179.9998         estimate D2E/DX2
!
 ! D63   D(22,14,15,9)         179.9999         estimate D2E/DX2
!
 ! D64   D(22,14,15,23)         -0.0001         estimate D2E/DX2
!
 ---------------------------------------------------------------------
-----------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
 Number of steps in this run= 145 maximum allowed number of steps=
150.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -5.554698   -0.913406    0.057466
    2          6             0       -4.197755   -0.912961    0.061517
    3          6             0       -3.498743    0.299680    0.055852
    4          6             0       -4.207386    1.504664    0.046032
    5          6             0       -5.606911    1.483183    0.041990
    6          6             0       -6.266841    0.297530    0.047600
    7          6             0       -2.097380    0.308877    0.059979
    8          6             0       -3.518216    2.724882    0.040289
    9          6             0       -2.116853    2.734079    0.044416
   10          6             0       -1.408210    1.529096    0.054237
   11          6             0       -0.008685    1.550576    0.058280
   12          1             0        0.540628    0.632372    0.065793
   13          6             0        0.651245    2.736229    0.052672
   14          6             0       -0.060898    3.947165    0.042800
   15          6             0       -1.417841    3.946720    0.038751
   16          1             0       -1.554979   -0.613427    0.067496
   17          1             0       -6.085838   -1.842261    0.061817
   18          1             0       -3.662296   -1.839313    0.069040
   19          1             0       -6.156223    2.401387    0.034479
   20          1             0       -7.336761    0.284823    0.044488
   21          1             0        1.721165    2.748937    0.055787
   22          1             0        0.470242    4.876020    0.038447
   23          1             0       -1.953300    4.873072    0.031229
   24          6             0       -4.298868    4.052311    0.029472
   25          7             0       -4.880097    5.040642    0.021418
 ---------------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356949	0.000000			
3	C	2.387159	1.399696	0.000000		
4	C	2.768111	2.417694	1.397947	0.000000	
5	C	2.397207	2.779858	2.417694	1.399696	0.000000
6	C	1.404853	2.397207	2.768111	2.387159	1.356949
7	C	3.667019	2.429911	1.401400	2.425331	3.700828
8	C	4.169495	3.700828	2.425330	1.401400	2.429911
9	C	5.012295	4.198970	2.799295	2.425242	3.707460
10	C	4.812399	3.707460	2.425242	2.799295	4.198970
11	C	6.068729	4.859767	3.707460	4.198970	5.598656
12	H	6.288282	4.984008	4.053061	4.827517	6.206181
13	C	7.199555	6.068729	4.812399	5.012295	6.382379
14	C	7.335339	6.382379	5.012295	4.812399	6.068729
15	C	6.382379	5.598656	4.198970	3.707460	4.859767
16	H	4.010965	2.659703	2.147585	3.394412	4.562300
17	H	1.070000	2.104389	3.358720	3.838063	3.359812
18	H	2.106804	1.070000	2.145277	3.388190	3.849836
19	H	3.369008	3.849836	3.388190	2.145277	1.070000
20	H	2.147480	3.359812	3.838063	3.358720	2.104389
21	H	8.145609	6.960111	5.765961	6.057725	7.436600
22	H	8.355699	7.436600	6.057725	5.765961	6.960111
23	H	6.815723	6.206180	4.827517	4.053060	4.984008
24	C	5.122132	4.966405	3.837073	2.549343	2.882976
25	N	5.992251	5.992712	4.938223	3.599485	3.631005

		6	7	8	9	10
6	C	0.000000				
7	C	4.169495	0.000000			
8	C	3.667019	2.802900	0.000000		
9	C	4.812399	2.425330	1.401400	0.000000	
10	C	5.012295	1.401400	2.425330	1.397947	0.000000
11	C	6.382379	2.429911	3.700828	2.417694	1.399696
12	H	6.815723	2.657774	4.566559	3.388190	2.145277
13	C	7.335339	3.667019	4.169495	2.768111	2.387159
14	C	7.199555	4.169495	3.667019	2.387159	2.768111
15	C	6.068729	3.700828	2.429911	1.399696	2.417694
16	H	4.799155	1.070000	3.872900	3.394412	2.147585
17	H	2.147480	4.531577	5.239460	6.057725	5.765961
18	H	3.369008	2.657774	4.566559	4.827517	4.053061
19	H	2.106804	4.566559	2.657774	4.053060	4.827517
20	H	1.070000	5.239460	4.531578	5.765961	6.057725
21	H	8.355699	4.531578	5.239460	3.838063	3.358720
22	H	8.145608	5.239460	4.531577	3.358720	3.838063
23	H	6.288282	4.566559	2.657774	2.145277	3.388190
24	C	4.239295	4.342900	1.540000	2.549343	3.837073
25	N	4.941746	5.489500	2.686600	3.599484	4.938222

		11	12	13	14	15
11	C	0.000000				
12	H	1.070000	0.000000			
13	C	1.356949	2.106804	0.000000		

14	C	2.397207	3.369008	1.404853	0.000000	
15	C	2.779858	3.849836	2.397207	1.356949	0.000000
16	H	2.659703	2.437947	4.010965	4.799155	4.562300
17	H	6.960111	7.073462	8.145609	8.355699	7.436600
18	H	4.984008	4.875839	6.288282	6.815723	6.206181
19	H	6.206181	6.926630	6.815723	6.288282	4.984008
20	H	7.436601	7.885081	8.355699	8.145609	6.960111
21	H	2.104389	2.423555	1.070000	2.147480	3.359812
22	H	3.359812	4.244320	2.147480	1.070000	2.104389
23	H	3.849836	4.919798	3.369008	2.106804	1.070000
24	C	4.966405	5.926046	5.122131	4.239295	2.882976
25	N	5.992710	6.987065	5.992249	4.941744	3.631003

		16	17	18	19	20
16	H	0.000000				
17	H	4.694544	0.000000			
18	H	2.437947	2.423554	0.000000		
19	H	5.501059	4.244320	4.919798	0.000000	
20	H	5.851187	2.467710	4.244320	2.423555	0.000000
21	H	4.694545	9.056955	7.073462	7.885081	9.387120
22	H	5.851187	9.387120	7.885081	7.073462	9.056954
23	H	5.501059	7.885081	6.926630	4.875838	7.073462
24	C	5.412900	6.159568	5.926046	2.485024	4.839730
25	N	6.559500	6.987832	6.987066	2.931609	5.352901

		21	22	23	24	25
21	H	0.000000				
22	H	2.467710	0.000000			
23	H	4.244320	2.423554	0.000000		
24	C	6.159568	4.839730	2.485023	0.000000	
25	N	6.987830	5.352898	2.931607	1.146600	0.000000

Stoichiometry C15H9N
Framework group C1[X(C15H9N)]
Deg. of freedom 69
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.599778	-1.115573	-0.000001
2	6	0	-2.429884	-1.803076	0.000000
3	6	0	-1.212621	-1.112121	0.000000
4	6	0	-1.212621	0.285827	0.000000
5	6	0	-2.429883	0.976782	0.000000
6	6	0	-3.599777	0.289280	0.000001
7	6	0	0.000000	-1.814597	0.000000
8	6	0	0.000000	0.988303	0.000000
9	6	0	1.212621	0.285826	0.000000
10	6	0	1.212621	-1.112121	0.000000
11	6	0	2.429883	-1.803076	0.000000
12	1	0	2.437919	-2.873046	0.000002

```
   13          6             0        3.599777   -1.115574    0.000002
   14          6             0        3.599777    0.289279   -0.000001
   15          6             0        2.429883    0.976781    0.000000
   16          1             0        0.000000   -2.884597    0.000000
   17          1             0       -4.528478   -1.647001   -0.000002
   18          1             0       -2.437920   -2.873046    0.000000
   19          1             0       -2.437919    2.046752    0.000000
   20          1             0       -4.528477    0.820708    0.000004
   21          1             0        4.528477   -1.647003    0.000003
   22          1             0        4.528477    0.820707   -0.000003
   23          1             0        2.437919    2.046751    0.000000
   24          6             0        0.000000    2.528303    0.000000
   25          7             0        0.000002    3.674903    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9688938      0.4668099
0.3150296
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   322 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   322 basis functions,   548 primitive gaussians,   322 cartesian
basis functions
    53 alpha electrons       53 beta electrons
       nuclear repulsion energy       941.7253926348 Hartrees.
 NAtoms=   25 NActive=   25 NUniq=   25 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   322 RedAO= T  NBF=   322
 NBsUse=   315 1.00D-06 NBFU=   315
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 4.17D+03 ExpMxC= 6.27D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -631.776515848     A.U. after   17 cycles
            Convg  =    0.6457D-08             -V/T =  2.0082
            S**2   =   0.0000


**********************************************************************

           Population analysis using the SCF density.


**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -14.34596 -10.25017 -10.24221 -10.22344 -
10.22343
 Alpha  occ. eigenvalues --  -10.21933 -10.21852 -10.21834 -10.20703 -
10.20703
 Alpha  occ. eigenvalues --  -10.20648 -10.20648 -10.20553 -10.20553 -
10.20317
 Alpha  occ. eigenvalues --  -10.20317  -0.92772  -0.91391  -0.88518
-0.83171
 Alpha  occ. eigenvalues --   -0.81876  -0.78094  -0.76921  -0.73192
-0.67598
 Alpha  occ. eigenvalues --   -0.64910  -0.64350  -0.61864  -0.56785
-0.55333
 Alpha  occ. eigenvalues --   -0.54628  -0.50408  -0.48475  -0.48460
-0.47954
 Alpha  occ. eigenvalues --   -0.45243  -0.45090  -0.43786  -0.42963
-0.42438
 Alpha  occ. eigenvalues --   -0.39751  -0.39110  -0.37671  -0.37376
-0.37107
 Alpha  occ. eigenvalues --   -0.35921  -0.35897  -0.34388  -0.32608
-0.31551
 Alpha  occ. eigenvalues --   -0.28069  -0.26830  -0.21819
 Alpha virt. eigenvalues --   -0.09416  -0.03259  -0.01785  -0.01723
-0.00156
 Alpha virt. eigenvalues --    0.00539   0.01238   0.02059   0.02657
0.03110
 Alpha virt. eigenvalues --    0.03162   0.04018   0.04887   0.04906
0.05047
 Alpha virt. eigenvalues --    0.05914   0.06273   0.06965   0.07071
0.07662
 Alpha virt. eigenvalues --    0.08308   0.09146   0.09399   0.09591
0.11280
 Alpha virt. eigenvalues --    0.11309   0.11762   0.12173   0.12353
0.12430
 Alpha virt. eigenvalues --    0.13076   0.13545   0.14247   0.14706
0.14877
 Alpha virt. eigenvalues --    0.15625   0.17070   0.17546   0.17750
0.18039
 Alpha virt. eigenvalues --    0.18066   0.18476   0.18978   0.19026
0.19315
 Alpha virt. eigenvalues --    0.19480   0.20346   0.20636   0.21358
0.22372
 Alpha virt. eigenvalues --    0.22688   0.23039   0.23226   0.23741
0.24256
 Alpha virt. eigenvalues --    0.24603   0.25084   0.25087   0.25753
0.25832
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.26620   0.27193   0.27319   0.27322
0.28173
 Alpha virt. eigenvalues --    0.28354   0.28572   0.29271   0.29422
0.30837
 Alpha virt. eigenvalues --    0.31178   0.31242   0.31396   0.31735
0.33463
 Alpha virt. eigenvalues --    0.33734   0.34253   0.35626   0.36253
0.37681
 Alpha virt. eigenvalues --    0.38676   0.39148   0.41591   0.41787
0.44841
 Alpha virt. eigenvalues --    0.48224   0.49023   0.50825   0.58749
0.59763
 Alpha virt. eigenvalues --    0.62828   0.63440   0.64028   0.65414
0.65819
 Alpha virt. eigenvalues --    0.65987   0.67371   0.70388   0.70574
0.70834
 Alpha virt. eigenvalues --    0.70907   0.71556   0.71884   0.72086
0.72957
 Alpha virt. eigenvalues --    0.73091   0.73311   0.75935   0.76185
0.77273
 Alpha virt. eigenvalues --    0.77370   0.77622   0.77656   0.79092
0.79180
 Alpha virt. eigenvalues --    0.79314   0.80182   0.81898   0.82025
0.85330
 Alpha virt. eigenvalues --    0.87066   0.88268   0.89281   0.89944
0.91266
 Alpha virt. eigenvalues --    0.91547   0.91830   0.94787   0.95452
0.95662
 Alpha virt. eigenvalues --    1.00373   1.00710   1.03299   1.03971
1.04058
 Alpha virt. eigenvalues --    1.06065   1.07565   1.07965   1.10538
1.11090
 Alpha virt. eigenvalues --    1.12171   1.12742   1.15598   1.17203
1.18541
 Alpha virt. eigenvalues --    1.18880   1.19377   1.19547   1.21980
1.22177
 Alpha virt. eigenvalues --    1.24593   1.24693   1.25456   1.26312
1.31834
 Alpha virt. eigenvalues --    1.32598   1.32766   1.35343   1.37409
1.37882
 Alpha virt. eigenvalues --    1.38911   1.42022   1.44486   1.45030
1.46725
 Alpha virt. eigenvalues --    1.47364   1.48183   1.48341   1.48538
1.50227
 Alpha virt. eigenvalues --    1.51457   1.54364   1.55516   1.58570
1.58867
 Alpha virt. eigenvalues --    1.64353   1.68324   1.71759   1.78947
1.80839
 Alpha virt. eigenvalues --    1.81482   1.82675   1.86171   1.86884
1.88796
 Alpha virt. eigenvalues --    1.90603   1.94581   1.94719   1.95244
1.95650
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    1.96651   1.97343   1.97989   1.98938
2.00003
 Alpha virt. eigenvalues --    2.01329   2.05646   2.07183   2.07588
2.08523
 Alpha virt. eigenvalues --    2.10533   2.12245   2.17986   2.18761
2.18998
 Alpha virt. eigenvalues --    2.21773   2.22697   2.25919   2.27600
2.29095
 Alpha virt. eigenvalues --    2.29368   2.30005   2.32729   2.33753
2.33940
 Alpha virt. eigenvalues --    2.38554   2.41459   2.41678   2.46470
2.51698
 Alpha virt. eigenvalues --    2.57708   2.62022   2.62985   2.64921
2.68073
 Alpha virt. eigenvalues --    2.69652   2.72891   2.73219   2.74126
2.76800
 Alpha virt. eigenvalues --    2.77021   2.77950   2.81669   2.84406
2.86537
 Alpha virt. eigenvalues --    2.87167   2.93371   2.97109   2.99704
3.07835
 Alpha virt. eigenvalues --    3.12292   3.17113   3.26146   3.39130
3.52633
 Alpha virt. eigenvalues --    3.56135   4.22698   4.24045   4.25483
4.25889
 Alpha virt. eigenvalues --    4.30390   4.30636   4.31667   4.31960
4.35852
 Alpha virt. eigenvalues --    4.40273   4.42343   4.44982   4.49299
4.62628
 Alpha virt. eigenvalues --    4.68619   4.93363
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C    6.096896   0.053369  -0.467226   0.600664  -1.122204
1.176571
     2  C    0.053369   7.247611  -0.110802  -1.231007   1.808380  -
1.352244
     3  C   -0.467226  -0.110802   8.119131   0.066032   1.233851  -
0.422166
     4  C    0.600664  -1.231007   0.066032  10.267350  -3.853329
1.027413
     5  C   -1.122204   1.808380   1.233851  -3.853329  12.121160  -
2.882737
     6  C    1.176571  -1.352244  -0.422166   1.027413  -2.882737
8.475923
     7  C   -0.169255   0.001263   0.484658  -1.448925   1.016438  -
0.568454
     8  C    0.087773  -0.404384  -0.439259   1.572901  -1.468392
0.469629
     9  C   -0.020293  -0.125120  -1.052923   0.205831  -0.428653
0.351768
    10  C   -0.089168   0.248998  -1.112541  -1.052924   0.058703  -
0.111974
```

This journal is © The Royal Society of Chemistry 2014

11	C	-0.018105	-0.123319	0.248997	-0.125121	-0.123398	0.024277
12	H	0.000800	0.004567	-0.011467	0.000178	0.000291	-0.000041
13	C	0.021277	-0.018105	-0.089168	-0.020293	-0.026663	-0.007283
14	C	-0.007283	0.024277	-0.111975	0.351766	0.100022	-0.045009
15	C	-0.026663	-0.123398	0.058704	-0.428651	-0.359046	0.100022
16	H	-0.000976	0.001664	-0.046982	0.007366	0.002843	0.001472
17	H	0.311355	-0.025521	0.010470	0.024410	-0.007651	-0.002972
18	H	0.020705	0.270313	-0.050966	0.065423	-0.036456	0.010543
19	H	0.018939	-0.018601	0.020737	-0.088369	0.289157	0.045829
20	H	-0.026585	0.011472	0.014038	-0.020881	0.021667	0.303852
21	H	-0.000003	0.000080	-0.002523	0.000792	-0.000037	-0.000007
22	H	0.000004	-0.000005	0.001414	-0.001732	-0.000099	0.000004
23	H	0.000016	-0.000614	-0.004453	0.001640	0.006658	0.001307
24	C	0.009288	-0.110937	-0.820739	-0.618655	0.133326	-0.002310
25	N	-0.000562	0.004660	0.047552	-0.018272	0.026025	0.036131

		7	8	9	10	11	12
1	C	-0.169255	0.087773	-0.020293	-0.089168	-0.018105	0.000800
2	C	0.001263	-0.404384	-0.125120	0.248998	-0.123319	0.004567
3	C	0.484658	-0.439259	-1.052923	-1.112541	0.248997	-0.011467
4	C	-1.448925	1.572901	0.205831	-1.052924	-0.125121	0.000178
5	C	1.016438	-1.468392	-0.428653	0.058703	-0.123398	0.000291
6	C	-0.568454	0.469629	0.351768	-0.111974	0.024277	-0.000041
7	C	7.705873	-0.612746	-1.448923	0.484662	0.001260	-0.006109
8	C	-0.612746	7.406202	1.572899	-0.439261	-0.404385	0.008420
9	C	-1.448923	1.572899	10.267343	0.066031	-1.231000	0.065423
10	C	0.484662	-0.439261	0.066031	8.119122	-0.110798	-0.050966

This journal is © The Royal Society of Chemistry 2014

11	C	0.001260	-0.404385	-1.231000	-0.110798	7.247611	0.270314
12	H	-0.006109	0.008420	0.065423	-0.050966	0.270314	0.540675
13	C	-0.169255	0.087773	0.600663	-0.467225	0.053368	0.020705
14	C	-0.568452	0.469630	1.027411	-0.422169	-1.352241	0.010543
15	C	1.016435	-1.468392	-3.853323	1.233854	1.808376	-0.036456
16	H	0.345436	-0.000708	0.007366	-0.046983	0.001664	0.003999
17	H	-0.014583	0.001071	0.000792	-0.002523	0.000080	0.000000
18	H	-0.006109	0.008420	0.000178	-0.011467	0.004567	0.000002
19	H	0.004848	-0.007110	0.001640	-0.004453	-0.000614	0.000000
20	H	0.003194	-0.006215	-0.001732	0.001414	-0.000005	0.000000
21	H	-0.014583	0.001071	0.024410	0.010470	-0.025521	-0.005155
22	H	0.003194	-0.006215	-0.020881	0.014038	0.011472	-0.000190
23	H	0.004848	-0.007110	-0.088369	0.020737	-0.018601	0.000021
24	C	-0.036600	-0.961174	-0.618660	-0.820738	-0.110940	0.000299
25	N	-0.006661	0.210187	-0.018271	0.047552	0.004661	0.000000

		13	14	15	16	17	18
1	C	0.021277	-0.007283	-0.026663	-0.000976	0.311355	0.020705
2	C	-0.018105	0.024277	-0.123398	0.001664	-0.025521	0.270313
3	C	-0.089168	-0.111975	0.058704	-0.046982	0.010470	-0.050966
4	C	-0.020293	0.351766	-0.428651	0.007366	0.024410	0.065423
5	C	-0.026663	0.100022	-0.359046	0.002843	-0.007651	-0.036456
6	C	-0.007283	-0.045009	0.100022	0.001472	-0.002972	0.010543
7	C	-0.169255	-0.568452	1.016435	0.345436	-0.014583	-0.006109
8	C	0.087773	0.469630	-1.468392	-0.000708	0.001071	0.008420
9	C	0.600663	1.027411	-3.853323	0.007366	0.000792	0.000178
10	C	-0.467225	-0.422169	1.233854	-0.046983	-0.002523	-0.011467

This journal is © The Royal Society of Chemistry 2014

11	C	0.053368	-1.352241	1.808376	0.001664	0.000080	0.004567
12	H	0.020705	0.010543	-0.036456	0.003999	0.000000	0.000002
13	C	6.096897	1.176570	-1.122203	-0.000976	-0.000003	0.000800
14	C	1.176570	8.475912	-2.882728	0.001472	-0.000007	-0.000041
15	C	-1.122203	-2.882728	12.121147	0.002843	-0.000037	0.000291
16	H	-0.000976	0.001472	0.002843	0.525711	-0.000015	0.003999
17	H	-0.000003	-0.000007	-0.000037	-0.000015	0.533206	-0.005155
18	H	0.000800	-0.000041	0.000291	0.003999	-0.005155	0.540675
19	H	0.000016	0.001307	0.006658	0.000001	-0.000189	0.000021
20	H	0.000004	0.000004	-0.000099	0.000000	-0.004514	-0.000190
21	H	0.311355	-0.002972	-0.007651	-0.000015	0.000000	0.000000
22	H	-0.026585	0.303852	0.021667	0.000000	0.000000	0.000000
23	H	0.018939	0.045829	0.289157	0.000001	0.000000	0.000000
24	C	0.009288	-0.002307	0.133325	0.000888	0.000008	0.000299
25	N	-0.000562	0.036131	0.026024	0.000011	0.000003	0.000000

		19	20	21	22	23	24
1	C	0.018939	-0.026585	-0.000003	0.000004	0.000016	0.009288
2	C	-0.018601	0.011472	0.000080	-0.000005	-0.000614	-0.110937
3	C	0.020737	0.014038	-0.002523	0.001414	-0.004453	-0.820739
4	C	-0.088369	-0.020881	0.000792	-0.001732	0.001640	-0.618655
5	C	0.289157	0.021667	-0.000037	-0.000099	0.006658	0.133326
6	C	0.045829	0.303852	-0.000007	0.000004	0.001307	-0.002310
7	C	0.004848	0.003194	-0.014583	0.003194	0.004848	-0.036600
8	C	-0.007110	-0.006215	0.001071	-0.006215	-0.007110	-0.961174
9	C	0.001640	-0.001732	0.024410	-0.020881	-0.088369	-0.618660
10	C	-0.004453	0.001414	0.010470	0.014038	0.020737	-0.820738

This journal is © The Royal Society of Chemistry 2014

```
    11  C   -0.000614  -0.000005  -0.025521   0.011472  -0.018601  -
0.110940
    12  H    0.000000   0.000000  -0.005155  -0.000190   0.000021
0.000299
    13  C    0.000016   0.000004   0.311355  -0.026585   0.018939
0.009288
    14  C    0.001307   0.000004  -0.002972   0.303852   0.045829  -
0.002307
    15  C    0.006658  -0.000099  -0.007651   0.021667   0.289157
0.133325
    16  H    0.000001   0.000000  -0.000015   0.000000   0.000001
0.000888
    17  H   -0.000189  -0.004514   0.000000   0.000000   0.000000
0.000008
    18  H    0.000021  -0.000190   0.000000   0.000000   0.000000
0.000299
    19  H    0.507834  -0.004654   0.000000   0.000000   0.000000
0.011090
    20  H   -0.004654   0.528203   0.000000   0.000000   0.000000  -
0.003805
    21  H    0.000000   0.000000   0.533206  -0.004514  -0.000189
0.000008
    22  H    0.000000   0.000000  -0.004514   0.528203  -0.004654  -
0.003805
    23  H    0.000000   0.000000  -0.000189  -0.004654   0.507834
0.011091
    24  C    0.011090  -0.003805   0.000008  -0.003805   0.011091
10.597210
    25  N    0.004748   0.000067   0.000003   0.000067   0.004748  -
0.218593
              25
     1  C   -0.000562
     2  C    0.004660
     3  C    0.047552
     4  C   -0.018272
     5  C    0.026025
     6  C    0.036131
     7  C   -0.006661
     8  C    0.210187
     9  C   -0.018271
    10  C    0.047552
    11  C    0.004661
    12  H    0.000000
    13  C   -0.000562
    14  C    0.036131
    15  C    0.026024
    16  H    0.000011
    17  H    0.000003
    18  H    0.000000
    19  H    0.004748
    20  H    0.000067
    21  H    0.000003
```

This journal is © The Royal Society of Chemistry 2014

```
   22  H    0.000067
   23  H    0.004748
   24  C   -0.218593
   25  N    7.344359
Mulliken atomic charges:
             1
    1  C   -0.449333
    2  C   -0.032599
    3  C    0.437605
    4  C    0.716392
    5  C   -0.509856
    6  C   -0.629543
    7  C   -0.001455
    8  C    0.329376
    9  C    0.716394
   10  C    0.437606
   11  C   -0.032598
   12  H    0.184145
   13  C   -0.449334
   14  C   -0.629543
   15  C   -0.509857
   16  H    0.189917
   17  H    0.181775
   18  H    0.184145
   19  H    0.211162
   20  H    0.184762
   21  H    0.181775
   22  H    0.184762
   23  H    0.211162
   24  C   -0.576856
   25  N   -0.530008
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  C   -0.267558
    2  C    0.151547
    3  C    0.437605
    4  C    0.716392
    5  C   -0.298694
    6  C   -0.444781
    7  C    0.188462
    8  C    0.329376
    9  C    0.716394
   10  C    0.437606
   11  C    0.151547
   12  H    0.000000
   13  C   -0.267558
   14  C   -0.444781
   15  C   -0.298694
   16  H    0.000000
   17  H    0.000000
   18  H    0.000000
```

```
   19  H    0.000000
   20  H    0.000000
   21  H    0.000000
   22  H    0.000000
   23  H    0.000000
   24  C   -0.576856
   25  N   -0.530008
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=  3326.3716
 Charge=     0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=    -4.7422    Z=     0.0000  Tot=     4.7422
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=   -75.6889   YY=  -100.5767   ZZ=   -97.3830
   XY=     0.0000   XZ=     0.0000   YZ=     0.0000
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=    15.5273   YY=    -9.3605   ZZ=    -6.1668
   XY=     0.0000   XZ=     0.0000   YZ=     0.0000
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=     0.0000  YYY=  -103.3669  ZZZ=     0.0000  XYY=     0.0000
  XXY=    -2.3749  XXZ=     0.0000  XZZ=     0.0000  YZZ=     2.8495
  YYZ=     0.0000  XYZ=    -0.0001
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX= -2696.1309 YYYY= -1794.9217 ZZZZ=  -116.1018 XXXY=     0.0000
 XXXZ=    -0.0001 YYYX=    -0.0002 YYYZ=     0.0000 ZZZX=     0.0000
 ZZZY=     0.0000 XXYY=  -699.3605 XXZZ=  -592.3363 YYZZ=  -289.1797
 XXYZ=     0.0000 YYXZ=     0.0001 ZZXY=     0.0000
 N-N= 9.417253926348D+02 E-N=-3.346216725821D+03  KE=
6.266425406729D+02
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.003761257   -0.008166725    0.000041185
    2          6          -0.008836930   -0.009269407    0.000032723
    3          6           0.033881286   -0.015998040    0.000203564
    4          6          -0.009876006    0.033941975   -0.000246602
    5          6          -0.012964392   -0.002431840   -0.000023022
    6          6          -0.006810641   -0.000332650   -0.000018391
    7          6          -0.010459114    0.017783952   -0.000144926
    8          6          -0.022688601    0.038579912   -0.000314416
    9          6          -0.024863030    0.025128487   -0.000234835
   10          6          -0.002486523   -0.037385281    0.000231466
   11          6           0.012396150    0.003217533    0.000016813
   12          1           0.004626089   -0.011653341    0.000088257
   13          6           0.008965361   -0.000682438    0.000030778
   14          6           0.003601058    0.005790318   -0.000026017
   15          6           0.008426569    0.010147959   -0.000039867
   16          1           0.006089615   -0.010354880    0.000084387
   17          1          -0.006874280   -0.010485539    0.000046545
   18          1           0.007935770   -0.009706967    0.000085721
```

```
   19          1          -0.004861249    0.010268346   -0.000080124
   20          1          -0.012370474   -0.000703793   -0.000032512
   21          1           0.012504921    0.000911116    0.000031547
   22          1           0.006627747    0.010468812   -0.000047106
   23          1          -0.006611077    0.009239302   -0.000078853
   24          6           0.049677270   -0.084471596    0.000688415
   25          7          -0.021268260    0.036164784   -0.000294731
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.084471596 RMS     0.016879656


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.056042617 RMS     0.010763143
 Search for a local minimum.
 Step number   1 out of a maximum of 145
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Second derivative matrix not updated -- first step.
     Eigenvalues ---    0.02070   0.02070   0.02070   0.02085
0.02085
     Eigenvalues ---    0.02088   0.02090   0.02093   0.02097
0.02227
     Eigenvalues ---    0.02229   0.02251   0.02256   0.02348
0.02348
     Eigenvalues ---    0.02376   0.02376   0.02423   0.02426
0.02499
     Eigenvalues ---    0.02502   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.22000   0.22000   0.22508   0.22589
0.23588
     Eigenvalues ---    0.24486   0.24559   0.25000   0.25000
0.25000
     Eigenvalues ---    0.25000   0.25000   0.28519   0.37230
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37230   0.37230
0.37230
     Eigenvalues ---    0.37230   0.37230   0.38433   0.41453
0.41543
     Eigenvalues ---    0.42889   0.42958   0.43700   0.45280
0.45319
     Eigenvalues ---    0.45389   0.45389   0.45635   0.45787
0.51539
     Eigenvalues ---    0.51549   0.52891   0.52923
1.369801000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 RFO step:  Lambda=-3.47138857D-02.
 Linear search not attempted -- first point.
 Iteration  1 RMS(Cart)=  0.05336719 RMS(Int)=  0.00019984
 Iteration  2 RMS(Cart)=  0.00025647 RMS(Int)=  0.00005200
 Iteration  3 RMS(Cart)=  0.00000011 RMS(Int)=  0.00005200
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.56426   0.01919   0.00000   0.03301   0.03296
2.59722
    R2        2.65479   0.01858   0.00000   0.03726   0.03717
2.69195
    R3        2.02201   0.01251   0.00000   0.03075   0.03075
2.05275
    R4        2.64504   0.02832   0.00000   0.05808   0.05812
2.70316
    R5        2.02201   0.01238   0.00000   0.03041   0.03041
2.05241
    R6        2.64174   0.03466   0.00000   0.07130   0.07140
2.71314
    R7        2.64826   0.00558   0.00000   0.01046   0.01041
2.65867
    R8        2.64504   0.02860   0.00000   0.05891   0.05897
2.70401
    R9        2.64826   0.01339   0.00000   0.02835   0.02841
2.67667
   R10        2.56426   0.02051   0.00000   0.03555   0.03551
2.59978
   R11        2.02201   0.01131   0.00000   0.02778   0.02778
2.04979
```

This journal is © The Royal Society of Chemistry 2014

R12	2.02201	0.01238	0.00000	0.03041	0.03041
2.05242					
R13	2.64826	0.00558	0.00000	0.01047	0.01041
2.65867					
R14	2.02201	0.01201	0.00000	0.02952	0.02952
2.05152					
R15	2.64826	0.01339	0.00000	0.02835	0.02841
2.67667					
R16	2.91018	-0.05604	0.00000	-0.17519	-0.17519
2.73499					
R17	2.64174	0.03466	0.00000	0.07130	0.07140
2.71314					
R18	2.64504	0.02860	0.00000	0.05891	0.05897
2.70401					
R19	2.64504	0.02832	0.00000	0.05808	0.05812
2.70316					
R20	2.02201	0.01238	0.00000	0.03041	0.03041
2.05241					
R21	2.56426	0.01919	0.00000	0.03301	0.03296
2.59722					
R22	2.65479	0.01858	0.00000	0.03726	0.03717
2.69195					
R23	2.02201	0.01251	0.00000	0.03075	0.03075
2.05275					
R24	2.56426	0.02051	0.00000	0.03555	0.03551
2.59978					
R25	2.02201	0.01238	0.00000	0.03041	0.03041
2.05242					
R26	2.02201	0.01131	0.00000	0.02778	0.02778
2.04979					
R27	2.16676	0.04196	0.00000	0.02987	0.02987
2.19663					
A1	2.10209	-0.00022	0.00000	-0.00502	-0.00516
2.09693					
A2	2.09055	0.00088	0.00000	0.00647	0.00654
2.09709					
A3	2.09055	-0.00066	0.00000	-0.00145	-0.00138
2.08917					
A4	2.09402	0.00425	0.00000	0.01566	0.01565
2.10966					
A5	2.09458	-0.00009	0.00000	0.00262	0.00263
2.09721					
A6	2.09458	-0.00416	0.00000	-0.01828	-0.01827
2.07631					
A7	2.08707	-0.00396	0.00000	-0.01080	-0.01065
2.07643					
A8	2.10025	0.00578	0.00000	0.01978	0.01970
2.11996					
A9	2.09586	-0.00182	0.00000	-0.00898	-0.00906
2.08680					
A10	2.08707	-0.00509	0.00000	-0.01593	-0.01582
2.07125					

This journal is © The Royal Society of Chemistry 2014

A11	2.09586	-0.00828	0.00000	-0.02857	-0.02855
2.06731					
A12	2.10025	0.01337	0.00000	0.04451	0.04437
2.14462					
A13	2.09402	0.00333	0.00000	0.01308	0.01310
2.10712					
A14	2.09458	-0.00278	0.00000	-0.01225	-0.01226
2.08232					
A15	2.09458	-0.00055	0.00000	-0.00083	-0.00084
2.09374					
A16	2.10209	0.00169	0.00000	0.00301	0.00288
2.10498					
A17	2.09055	-0.00141	0.00000	-0.00440	-0.00433
2.08621					
A18	2.09055	-0.00028	0.00000	0.00139	0.00145
2.09200					
A19	2.09147	0.00943	0.00000	0.03362	0.03357
2.12503					
A20	2.09586	-0.00471	0.00000	-0.01681	-0.01678
2.07908					
A21	2.09586	-0.00471	0.00000	-0.01681	-0.01678
2.07908					
A22	2.09147	0.01077	0.00000	0.04148	0.04164
2.13311					
A23	2.09586	-0.00539	0.00000	-0.02074	-0.02082
2.07504					
A24	2.09586	-0.00539	0.00000	-0.02074	-0.02082
2.07504					
A25	2.09586	-0.00828	0.00000	-0.02857	-0.02855
2.06731					
A26	2.10025	0.01337	0.00000	0.04451	0.04437
2.14462					
A27	2.08707	-0.00509	0.00000	-0.01593	-0.01582
2.07125					
A28	2.09586	-0.00182	0.00000	-0.00898	-0.00906
2.08680					
A29	2.10025	0.00578	0.00000	0.01978	0.01970
2.11996					
A30	2.08707	-0.00396	0.00000	-0.01080	-0.01065
2.07643					
A31	2.09458	-0.00416	0.00000	-0.01828	-0.01827
2.07631					
A32	2.09402	0.00425	0.00000	0.01566	0.01565
2.10966					
A33	2.09458	-0.00009	0.00000	0.00262	0.00263
2.09721					
A34	2.10209	-0.00022	0.00000	-0.00502	-0.00516
2.09693					
A35	2.09055	0.00088	0.00000	0.00647	0.00654
2.09709					
A36	2.09055	-0.00066	0.00000	-0.00145	-0.00138
2.08917					

This journal is © The Royal Society of Chemistry 2014

A37	2.10209	0.00169	0.00000	0.00301	0.00288
2.10498					
A38	2.09055	-0.00141	0.00000	-0.00440	-0.00433
2.08621					
A39	2.09055	-0.00028	0.00000	0.00139	0.00145
2.09200					
A40	2.09402	0.00333	0.00000	0.01308	0.01310
2.10712					
A41	2.09458	-0.00278	0.00000	-0.01225	-0.01226
2.08232					
A42	2.09458	-0.00055	0.00000	-0.00083	-0.00084
2.09374					
A43	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
A44	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D1	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D2	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D3	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D4	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D5	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D6	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D7	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D8	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D9	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D10	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D11	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D12	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D13	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D14	3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D15	3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D16	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D17	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D18	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					

This journal is © The Royal Society of Chemistry 2014

D19	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D20	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D21	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D22	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D23	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D24	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D25	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D26	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D27	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D28	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D29	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D30	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D31	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D32	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D33	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D34	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D35	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D36	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D37	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D38	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D39	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D40	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D41	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D42	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D43	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D44	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					

```
   D45       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D46        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D47        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D48        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D49        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D50       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D51        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D52        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D53        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D54        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D55       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D56        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D57        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D58       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D59       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D60        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D61        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D62        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D63        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D64        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.056043     0.000450     NO
 RMS     Force            0.010763     0.000300     NO
 Maximum Displacement     0.174894     0.001800     NO
 RMS     Displacement     0.053269     0.001200     NO
 Predicted change in Energy=-1.885286D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.606550	-0.961417	0.057619
2	6	0	-4.232285	-0.943477	0.061609
3	6	0	-3.514298	0.293717	0.055844
4	6	0	-4.251634	1.525608	0.045766
5	6	0	-5.681446	1.469971	0.041851
6	6	0	-6.337927	0.260976	0.047621
7	6	0	-2.107778	0.326559	0.059835
8	6	0	-3.529546	2.744147	0.040133
9	6	0	-2.113651	2.782929	0.044114
10	6	0	-1.395438	1.539791	0.054206
11	6	0	0.034767	1.565921	0.058311
12	1	0	0.577964	0.625458	0.065948
13	6	0	0.718407	2.758208	0.052731
14	6	0	0.005599	3.991522	0.042716
15	6	0	-1.370067	4.005437	0.038519
16	1	0	-1.557460	-0.609208	0.067461
17	1	0	-6.139925	-1.907713	0.062075
18	1	0	-3.674401	-1.875303	0.069233
19	1	0	-6.248773	2.394450	0.034247
20	1	0	-7.423709	0.235163	0.044544
21	1	0	1.804655	2.764392	0.055937
22	1	0	0.555902	4.927869	0.038372
23	1	0	-1.902253	4.950582	0.030887
24	6	0	-4.263204	3.991667	0.029966
25	7	0	-4.852447	4.993624	0.021800

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.374389	0.000000			
3	C	2.439853	1.430450	0.000000		
4	C	2.832178	2.469212	1.435730	0.000000	
5	C	2.432592	2.815172	2.465827	1.430900	0.000000
6	C	1.424520	2.425826	2.823831	2.439655	1.375743
7	C	3.728309	2.475181	1.406909	2.456427	3.752175
8	C	4.247994	3.754048	2.450528	1.416432	2.500841
9	C	5.120610	4.286609	2.856243	2.480288	3.801714
10	C	4.897909	3.770195	2.458103	2.856243	4.286595
11	C	6.181577	4.950234	3.770195	4.286609	5.717042
12	H	6.384862	5.059651	4.105699	4.912809	6.316170
13	C	7.337623	6.181577	4.897909	5.120610	6.528230
14	C	7.485188	6.504938	5.105253	4.919834	6.220989
15	C	6.528230	5.717042	4.286595	3.801714	5.001659
16	H	4.064391	2.695636	2.155139	3.437511	4.618539
17	H	1.086271	2.137485	3.426405	3.918368	3.408718
18	H	2.137410	1.086090	2.174962	3.449630	3.901261
19	H	3.416846	3.899837	3.448318	2.177977	1.084702
20	H	2.175785	3.402157	3.909866	3.424517	2.135471
21	H	8.295036	7.084699	5.864768	6.181693	7.597200

This journal is © The Royal Society of Chemistry 2014

22	H	8.524076	7.576277	6.167836	5.889638	7.131731
23	H	6.976694	6.337974	4.928053	4.153343	5.137808
24	C	5.132093	4.935342	3.773111	2.466136	2.893182
25	N	6.002705	5.969536	4.886812	3.519756	3.619914
		6	7	8	9	10
6	C	0.000000				
7	C	4.230675	0.000000			
8	C	3.748760	2.804736	0.000000		
9	C	4.919834	2.456427	1.416432	0.000000	
10	C	5.105253	1.406909	2.450528	1.435730	0.000000
11	C	6.504938	2.475181	3.754047	2.469212	1.430450
12	H	6.925513	2.702331	4.621812	3.449630	2.174962
13	C	7.485188	3.728309	4.247994	2.832178	2.439853
14	C	7.359165	4.230675	3.748759	2.439655	2.823831
15	C	6.220989	3.752175	2.500841	1.430900	2.465827
16	H	4.859061	1.085619	3.890354	3.437511	2.155139
17	H	2.177757	4.609792	5.334263	6.181693	5.864768
18	H	3.414458	2.702331	4.621812	4.912809	4.105699
19	H	2.135377	4.628679	2.741628	4.153343	4.928053
20	H	1.086093	5.316738	4.632443	5.889638	6.167836
21	H	8.518733	4.609792	5.334263	3.918368	3.426405
22	H	8.324954	5.316738	4.632443	3.424517	3.909866
23	H	6.455067	4.628679	2.741628	2.177977	3.448318
24	C	4.268822	4.252031	1.447295	2.466136	3.773111
25	N	4.960370	5.414439	2.609703	3.519755	4.886811
		11	12	13	14	15
11	C	0.000000				
12	H	1.086090	0.000000			
13	C	1.374388	2.137410	0.000000		
14	C	2.425826	3.414458	1.424520	0.000000	
15	C	2.815172	3.901261	2.432592	1.375743	0.000000
16	H	2.695636	2.466666	4.064391	4.859061	4.618539
17	H	7.084699	7.179624	8.295036	8.518733	7.597200
18	H	5.059651	4.933196	6.384862	6.925513	6.316170
19	H	6.337974	7.052282	6.976694	6.455067	5.137808
20	H	7.576277	8.011215	8.524076	8.324954	7.131731
21	H	2.137485	2.465747	1.086271	2.177757	3.408718
22	H	3.402157	4.302556	2.175785	1.086093	2.135471
23	H	3.899837	4.985920	3.416846	2.135377	1.084702
24	C	4.935342	5.896572	5.132093	4.268822	2.893182
25	N	5.969534	6.969375	6.002703	4.960368	3.619912
		16	17	18	19	20
16	H	0.000000				
17	H	4.762891	0.000000			
18	H	2.466666	2.465747	0.000000		
19	H	5.570591	4.303629	4.985920	0.000000	
20	H	5.926750	2.498064	4.302556	2.458271	0.000000
21	H	4.762891	9.216559	7.179624	8.061950	9.568691
22	H	5.926750	9.568691	8.011215	7.260981	9.257198
23	H	5.570591	8.061950	7.052282	5.042427	7.260981
24	C	5.337650	6.190783	5.896573	2.548256	4.909209
25	N	6.500057	7.020518	6.969376	2.950524	5.408777

This journal is © The Royal Society of Chemistry 2014

```
                    21         22         23         24         25
    21  H    0.000000
    22  H    2.498064   0.000000
    23  H    4.303629   2.458271   0.000000
    24  C    6.190783   4.909209   2.548256   0.000000
    25  N    7.020516   5.408774   2.950522   1.162408   0.000000
 Stoichiometry    C15H9N
 Framework group  C1[X(C15H9N)]
 Deg. of freedom    69
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -3.668812   -1.131030   -0.000001
    2          6             0       -2.475117   -1.812233    0.000000
    3          6             0       -1.229052   -1.109732    0.000000
    4          6             0       -1.240144    0.325956    0.000000
    5          6             0       -2.500829    1.002822    0.000000
    6          6             0       -3.679583    0.293449    0.000001
    7          6             0        0.000000   -1.794440    0.000000
    8          6             0        0.000000    1.010296    0.000000
    9          6             0        1.240144    0.325955    0.000000
   10          6             0        1.229051   -1.109732    0.000000
   11          6             0        2.475117   -1.812233    0.000000
   12          1             0        2.466598   -2.898290    0.000002
   13          6             0        3.668811   -1.131031    0.000001
   14          6             0        3.679583    0.293449   -0.000001
   15          6             0        2.500829    1.002821    0.000000
   16          1             0        0.000000   -2.880058    0.000000
   17          1             0       -4.608280   -1.676360   -0.000002
   18          1             0       -2.466599   -2.898289    0.000000
   19          1             0       -2.521213    2.087332    0.000000
   20          1             0       -4.628599    0.821622    0.000002
   21          1             0        4.608279   -1.676361    0.000001
   22          1             0        4.628599    0.821621   -0.000002
   23          1             0        2.521213    2.087331    0.000000
   24          6             0        0.000000    2.457591    0.000000
   25          7             0        0.000002    3.619999    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9801604      0.4474974
0.3072299
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   322 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   322 basis functions,   548 primitive gaussians,   322 cartesian
basis functions
```

This journal is © The Royal Society of Chemistry 2014

```
    53 alpha electrons       53 beta electrons
       nuclear repulsion energy       930.5465946185 Hartrees.
 NAtoms=   25 NActive=   25 NUniq=   25 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   322 RedAO= T  NBF=   322
 NBsUse=   315 1.00D-06 NBFU=   315
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 4.17D+03 ExpMxC= 6.27D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -631.795045244     A.U. after   15 cycles
             Convg  =    0.7889D-08             -V/T =  2.0099
             S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
```

This journal is © The Royal Society of Chemistry 2014

Number	Number	X	Y	Z
1	6	0.002865115	-0.000170355	0.000009748
2	6	-0.004443503	0.000020578	-0.000013483
3	6	0.007007943	-0.005168364	0.000054014
4	6	-0.003080144	0.003600605	-0.000032268
5	6	-0.000388356	-0.002741532	0.000016450
6	6	0.002500215	0.002057986	-0.000005770
7	6	-0.003851037	0.006548210	-0.000053357
8	6	-0.006162835	0.010479228	-0.000085407
9	6	-0.001649598	0.004441879	-0.000033292
10	6	0.001110706	-0.008636435	0.000058476
11	6	0.002141745	0.003893285	-0.000018274
12	1	-0.000398548	-0.001250015	0.000006744
13	6	-0.001243712	-0.002586690	0.000012624
14	6	-0.003013775	-0.001184723	-0.000001301
15	6	0.002584698	-0.000993129	0.000013980
16	1	0.000798684	-0.001358075	0.000011067
17	1	-0.000170610	-0.000173861	0.000000645
18	1	0.001286146	-0.000259265	0.000005477
19	1	0.000188534	0.001132742	-0.000006652
20	1	-0.000341333	0.000212336	-0.000002439
21	1	0.000234867	0.000064594	0.000000290
22	1	-0.000019662	0.000401506	-0.000002591
23	1	-0.001081582	0.000385803	-0.000005719
24	6	0.008232081	-0.013997773	0.000114080
25	7	-0.003106036	0.005281467	-0.000043043

Cartesian Forces: Max 0.013997773 RMS 0.003275383

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Internal Forces: Max 0.010112140 RMS 0.001437345
Search for a local minimum.
Step number 2 out of a maximum of 145
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Update second derivatives using D2CorX and points 1 2
Trust test= 9.83D-01 RLast= 2.94D-01 DXMaxT set to 4.24D-01
Eigenvalues --- 0.02070 0.02070 0.02070 0.02084
0.02085
Eigenvalues --- 0.02088 0.02089 0.02093 0.02097
0.02229
Eigenvalues --- 0.02231 0.02253 0.02257 0.02349
0.02349
Eigenvalues --- 0.02378 0.02378 0.02425 0.02428
0.02501
Eigenvalues --- 0.02504 0.15948 0.16000 0.16000
0.16000
Eigenvalues --- 0.16000 0.16000 0.16000 0.16000
0.16005

```
     Eigenvalues ---    0.21980   0.22000   0.22556   0.22581
0.23618
     Eigenvalues ---    0.24474   0.24558   0.25000   0.25000
0.25000
     Eigenvalues ---    0.25000   0.25440   0.27031   0.37119
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37230   0.37230
0.37230
     Eigenvalues ---    0.37230   0.37354   0.38670   0.41079
0.41603
     Eigenvalues ---    0.42942   0.42960   0.43790   0.44625
0.45327
     Eigenvalues ---    0.45389   0.45563   0.45632   0.47589
0.51576
     Eigenvalues ---    0.51590   0.52939   0.55821
1.356951000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 RFO step:  Lambda=-6.55120674D-04.
 Quartic linear search produced a step of  0.06672.
 Iteration  1 RMS(Cart)=  0.00532215 RMS(Int)=  0.00000867
 Iteration  2 RMS(Cart)=  0.00001322 RMS(Int)=  0.00000276
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000276
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.59722  -0.00271   0.00220  -0.00733  -0.00513
2.59209
```

This journal is © The Royal Society of Chemistry 2014

R2	2.69195	0.00080	0.00248	-0.00057	0.00190
2.69385					
R3	2.05275	0.00024	0.00205	-0.00105	0.00100
2.05375					
R4	2.70316	-0.00009	0.00388	-0.00314	0.00074
2.70390					
R5	2.05241	0.00088	0.00203	0.00082	0.00285
2.05526					
R6	2.71314	0.00446	0.00476	0.00684	0.01161
2.72475					
R7	2.65867	-0.00441	0.00069	-0.01139	-0.01070
2.64797					
R8	2.70401	-0.00193	0.00393	-0.00758	-0.00364
2.70037					
R9	2.67667	0.00001	0.00190	-0.00106	0.00084
2.67751					
R10	2.59978	-0.00219	0.00237	-0.00650	-0.00413
2.59565					
R11	2.04979	0.00087	0.00185	0.00092	0.00277
2.05256					
R12	2.05242	0.00034	0.00203	-0.00075	0.00128
2.05370					
R13	2.65867	-0.00441	0.00069	-0.01139	-0.01070
2.64797					
R14	2.05152	0.00158	0.00197	0.00285	0.00482
2.05634					
R15	2.67667	0.00001	0.00190	-0.00106	0.00084
2.67751					
R16	2.73499	-0.01011	-0.01169	-0.02752	-0.03921
2.69578					
R17	2.71314	0.00446	0.00476	0.00684	0.01161
2.72475					
R18	2.70401	-0.00193	0.00393	-0.00758	-0.00364
2.70037					
R19	2.70316	-0.00009	0.00388	-0.00314	0.00074
2.70390					
R20	2.05241	0.00088	0.00203	0.00082	0.00285
2.05526					
R21	2.59722	-0.00271	0.00220	-0.00733	-0.00513
2.59209					
R22	2.69195	0.00080	0.00248	-0.00057	0.00190
2.69385					
R23	2.05275	0.00024	0.00205	-0.00105	0.00100
2.05375					
R24	2.59978	-0.00219	0.00237	-0.00650	-0.00413
2.59565					
R25	2.05242	0.00034	0.00203	-0.00075	0.00128
2.05370					
R26	2.04979	0.00087	0.00185	0.00092	0.00277
2.05256					
R27	2.19663	0.00613	0.00199	0.00325	0.00524
2.20187					

This journal is © The Royal Society of Chemistry 2014

A1	2.09693	0.00014	-0.00034	-0.00022	-0.00057
2.09636					
A2	2.09709	-0.00001	0.00044	0.00028	0.00072
2.09781					
A3	2.08917	-0.00014	-0.00009	-0.00006	-0.00015
2.08902					
A4	2.10966	-0.00021	0.00104	-0.00179	-0.00075
2.10891					
A5	2.09721	0.00110	0.00018	0.00682	0.00700
2.10421					
A6	2.07631	-0.00089	-0.00122	-0.00503	-0.00625
2.07006					
A7	2.07643	-0.00040	-0.00071	0.00056	-0.00015
2.07628					
A8	2.11996	0.00047	0.00131	0.00046	0.00177
2.12172					
A9	2.08680	-0.00008	-0.00060	-0.00101	-0.00162
2.08518					
A10	2.07125	-0.00048	-0.00106	-0.00055	-0.00160
2.06965					
A11	2.06731	0.00035	-0.00190	0.00381	0.00190
2.06922					
A12	2.14462	0.00014	0.00296	-0.00325	-0.00030
2.14432					
A13	2.10712	-0.00028	0.00087	-0.00233	-0.00146
2.10566					
A14	2.08232	-0.00063	-0.00082	-0.00358	-0.00440
2.07792					
A15	2.09374	0.00091	-0.00006	0.00592	0.00586
2.09960					
A16	2.10498	0.00123	0.00019	0.00434	0.00453
2.10951					
A17	2.08621	-0.00039	-0.00029	-0.00048	-0.00077
2.08545					
A18	2.09200	-0.00084	0.00010	-0.00386	-0.00376
2.08823					
A19	2.12503	0.00139	0.00224	0.00306	0.00529
2.13033					
A20	2.07908	-0.00069	-0.00112	-0.00153	-0.00265
2.07643					
A21	2.07908	-0.00069	-0.00112	-0.00153	-0.00265
2.07643					
A22	2.13311	-0.00193	0.00278	-0.00865	-0.00586
2.12725					
A23	2.07504	0.00097	-0.00139	0.00432	0.00293
2.07797					
A24	2.07504	0.00097	-0.00139	0.00432	0.00293
2.07797					
A25	2.06731	0.00035	-0.00190	0.00381	0.00190
2.06922					
A26	2.14462	0.00014	0.00296	-0.00325	-0.00030
2.14432					

This journal is © The Royal Society of Chemistry 2014

```
   A27        2.07125  -0.00048  -0.00106  -0.00055  -0.00160
2.06965
   A28        2.08680  -0.00008  -0.00060  -0.00101  -0.00162
2.08518
   A29        2.11996   0.00047   0.00131   0.00046   0.00177
2.12172
   A30        2.07643  -0.00040  -0.00071   0.00056  -0.00015
2.07628
   A31        2.07631  -0.00089  -0.00122  -0.00503  -0.00625
2.07006
   A32        2.10966  -0.00021   0.00104  -0.00179  -0.00075
2.10891
   A33        2.09721   0.00110   0.00018   0.00682   0.00700
2.10421
   A34        2.09693   0.00014  -0.00034  -0.00022  -0.00057
2.09636
   A35        2.09709  -0.00001   0.00044   0.00028   0.00072
2.09781
   A36        2.08917  -0.00014  -0.00009  -0.00006  -0.00015
2.08902
   A37        2.10498   0.00123   0.00019   0.00434   0.00453
2.10951
   A38        2.08621  -0.00039  -0.00029  -0.00048  -0.00077
2.08545
   A39        2.09200  -0.00084   0.00010  -0.00386  -0.00376
2.08823
   A40        2.10712  -0.00028   0.00087  -0.00233  -0.00146
2.10566
   A41        2.08232  -0.00063  -0.00082  -0.00358  -0.00440
2.07792
   A42        2.09374   0.00091  -0.00006   0.00592   0.00586
2.09960
   A43        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   A44        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
    D1        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D2        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
    D3        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
    D4        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D5        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D6       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
    D7       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
    D8        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
```

This journal is © The Royal Society of Chemistry 2014

D9	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D10	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D11	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D12	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D13	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D14	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D15	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D16	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D17	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D18	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D19	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D20	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D21	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D22	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D23	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D24	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D25	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D26	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D27	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D28	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D29	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D30	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D31	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D32	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D33	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D34	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					

This journal is © The Royal Society of Chemistry 2014

D35	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D36	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D37	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D38	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D39	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D40	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D41	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D42	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D43	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D44	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D45	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D46	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D47	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D48	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D49	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D50	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D51	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D52	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D53	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D54	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D55	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D56	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D57	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D58	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D59	-3.14159	0.00000	0.00000	0.00000	0.00000
-3.14159					
D60	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					

```
   D61        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D62        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D63        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D64        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.010112     0.000450     NO
 RMS     Force            0.001437     0.000300     NO
 Maximum Displacement     0.020726     0.001800     NO
 RMS     Displacement     0.005327     0.001200     NO
 Predicted change in Energy=-4.036065D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -5.600273   -0.960858    0.057635
    2          6             0       -4.228725   -0.942782    0.061616
    3          6             0       -3.511628    0.295382    0.055842
    4          6             0       -4.253386    1.531784    0.045722
    5          6             0       -5.681122    1.472466    0.041837
    6          6             0       -6.331623    0.262723    0.047628
    7          6             0       -2.110860    0.331799    0.059793
    8          6             0       -3.534644    2.752816    0.040062
    9          6             0       -2.118196    2.787462    0.044071
   10          6             0       -1.398191    1.538266    0.054208
   11          6             0        0.032430    1.563148    0.058322
   12          1             0        0.569657    0.617529    0.065973
   13          6             0        0.714868    2.752994    0.052753
   14          6             0        0.001008    3.986862    0.042733
   15          6             0       -1.372405    4.006367    0.038506
   16          1             0       -1.559249   -0.606166    0.067437
   17          1             0       -6.134470   -1.907297    0.062090
   18          1             0       -3.663433   -1.871897    0.069244
   19          1             0       -6.247574    2.399201    0.034220
   20          1             0       -7.418076    0.236543    0.044551
   21          1             0        1.801641    2.759827    0.055956
   22          1             0        0.551958    4.923616    0.038389
   23          1             0       -1.906988    4.951843    0.030864
   24          6             0       -4.257785    3.982452    0.030041
   25          7             0       -4.848433    4.986798    0.021856
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
```

This journal is © The Royal Society of Chemistry 2014

2	C	1.371673	0.000000			
3	C	2.437331	1.430843	0.000000		
4	C	2.833286	2.474740	1.441873	0.000000	
5	C	2.434718	2.818381	2.468285	1.428973	0.000000
6	C	1.425526	2.423968	2.820197	2.435074	1.373558
7	C	3.721152	2.471824	1.401247	2.455724	3.748095
8	C	4.249530	3.760274	2.457592	1.416878	2.499334
9	C	5.116146	4.285950	2.855215	2.477048	3.797850
10	C	4.889083	3.763985	2.451812	2.855215	4.283455
11	C	6.172354	4.943394	3.763985	4.285949	5.714296
12	H	6.368627	5.045697	4.093991	4.908973	6.309020
13	C	7.326235	6.172354	4.889083	5.116146	6.522926
14	C	7.473587	6.495567	5.095666	4.911954	6.213598
15	C	6.522926	5.714296	4.283455	3.797850	4.998571
16	H	4.056572	2.690622	2.150512	3.439429	4.616406
17	H	1.086799	2.135920	3.425075	3.919952	3.410092
18	H	2.140438	1.087597	2.172630	3.454510	3.905967
19	H	3.421921	3.904530	3.451366	2.174702	1.086169
20	H	2.176774	3.400449	3.906907	3.419490	2.131788
21	H	8.284433	7.076345	5.856988	6.178312	7.592710
22	H	8.513364	7.567701	6.159025	5.881829	7.124728
23	H	6.971449	6.335457	4.925254	4.147603	5.133252
24	C	5.122436	4.925421	3.761901	2.450722	2.885491
25	N	5.995095	5.962008	4.878278	3.505963	3.611690

		6	7	8	9	10
6	C	0.000000				
7	C	4.221346	0.000000			
8	C	3.744825	2.808713	0.000000		
9	C	4.911954	2.455724	1.416877	0.000000	
10	C	5.095666	1.401247	2.457592	1.441873	0.000000
11	C	6.495567	2.471824	3.760274	2.474740	1.430843
12	H	6.910419	2.695709	4.626597	3.454510	2.172630
13	C	7.473587	3.721152	4.249530	2.833286	2.437331
14	C	7.346527	4.221346	3.744825	2.435074	2.820197
15	C	6.213598	3.748095	2.499334	1.428973	2.468285
16	H	4.850867	1.088168	3.896882	3.439429	2.150512
17	H	2.179005	4.604671	5.336313	6.178312	5.856988
18	H	3.417061	2.695709	4.626597	4.908973	4.093991
19	H	2.138173	4.624630	2.735885	4.147603	4.925253
20	H	1.086772	5.308092	4.627385	5.881829	6.159025
21	H	8.507972	4.604671	5.336313	3.919952	3.425075
22	H	8.313104	5.308092	4.627385	3.419490	3.906907
23	H	6.447133	4.624630	2.735885	2.174702	3.451366
24	C	4.258814	4.235261	1.426548	2.450722	3.761901
25	N	4.951505	5.400441	2.591728	3.505962	4.878277

		11	12	13	14	15
11	C	0.000000				
12	H	1.087597	0.000000			
13	C	1.371673	2.140437	0.000000		
14	C	2.423968	3.417061	1.425526	0.000000	
15	C	2.818381	3.905967	2.434718	1.373558	0.000000
16	H	2.690622	2.455539	4.056572	4.850867	4.616406

This journal is © The Royal Society of Chemistry 2014

17	H	7.076345	7.163803	8.284433	8.507972	7.592710
18	H	5.045697	4.910835	6.368627	6.910419	6.309020
19	H	6.335457	7.046275	6.971449	6.447133	5.133252
20	H	7.567701	7.996842	8.513364	8.313104	7.124728
21	H	2.135920	2.471301	1.086799	2.179005	3.410092
22	H	3.400449	4.306212	2.176774	1.086772	2.131788
23	H	3.904530	4.992122	3.421921	2.138173	1.086169
24	C	4.925421	5.884572	5.122436	4.258814	2.885491
25	N	5.962008	6.960471	5.995094	4.951504	3.611689

		16	17	18	19	20
16	H	0.000000				
17	H	4.756640	0.000000			
18	H	2.455539	2.471301	0.000000		
19	H	5.568996	4.308073	4.992122	0.000000	
20	H	5.919166	2.498799	4.306212	2.459120	0.000000
21	H	4.756640	9.206734	7.163803	8.057318	9.558779
22	H	5.919166	9.558779	7.996842	7.253022	9.246087
23	H	5.568996	8.057318	7.046275	5.035541	7.253022
24	C	5.323429	6.181595	5.884572	2.542826	4.900968
25	N	6.488609	7.013135	6.960472	2.941668	5.400788

		21	22	23	24	25
21	H	0.000000				
22	H	2.498799	0.000000			
23	H	4.308073	2.459120	0.000000		
24	C	6.181595	4.900968	2.542826	0.000000	
25	N	7.013133	5.400786	2.941666	1.165180	0.000000

Stoichiometry C15H9N
Framework group C1[X(C15H9N)]
Deg. of freedom 69
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.663118	-1.133792	0.000000
2	6	0	2.471697	-1.813500	0.000000
3	6	0	1.225906	-1.109712	0.000000
4	6	0	1.238524	0.332105	0.000000
5	6	0	2.499285	1.004746	0.000000
6	6	0	3.673263	0.291698	0.000000
7	6	0	0.000000	-1.788422	0.000000
8	6	0	0.000000	1.020291	0.000000
9	6	0	-1.238524	0.332105	0.000000
10	6	0	-1.225906	-1.109713	0.000000
11	6	0	-2.471697	-1.813500	0.000000
12	1	0	-2.455417	-2.900975	-0.000001
13	6	0	-3.663118	-1.133793	0.000000
14	6	0	-3.673263	0.291697	0.000000
15	6	0	-2.499286	1.004746	0.000000

```
   16          1             0        0.000000   -2.876591    0.000000
   17          1             0        4.603367   -1.678828    0.000001
   18          1             0        2.455418   -2.900975    0.000000
   19          1             0        2.517770    2.090758    0.000000
   20          1             0        4.623044    0.819894    0.000000
   21          1             0       -4.603367   -1.678829    0.000000
   22          1             0       -4.623044    0.819893    0.000001
   23          1             0       -2.517771    2.090758    0.000000
   24          6             0        0.000000    2.446839    0.000000
   25          7             0       -0.000001    3.612019    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9820281      0.4488211
0.3080373
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   322 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   322 basis functions,   548 primitive gaussians,   322 cartesian
basis functions
    53 alpha electrons       53 beta electrons
       nuclear repulsion energy       931.4601810299 Hartrees.
 NAtoms=   25 NActive=   25 NUniq=   25 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   322 RedAO= T  NBF=   322
 NBsUse=   315 1.00D-06 NBFU=   315
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 4.17D+03 ExpMxC= 6.27D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Restarting incremental Fock formation.
 SCF Done:  E(RB+HF-LYP) =  -631.795408810     A.U. after   20 cycles
            Convg  =    0.9121D-08             -V/T =  2.0098
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6           0.000287096   -0.000100338    0.000001469
    2          6          -0.000983391    0.000192533   -0.000004163
    3          6           0.000615191   -0.001142296    0.000009134
    4          6          -0.000493480   -0.000587047    0.000002285
    5          6           0.000307279   -0.000457432    0.000003833
    6          6           0.000089083    0.000141108   -0.000000604
    7          6          -0.000587800    0.000999479   -0.000008139
    8          6           0.000685797   -0.001166176    0.000009504
    9          6           0.000752901    0.000145916    0.000001312
   10          6           0.000699305   -0.001092824    0.000009077
   11          6           0.000309693    0.000952978   -0.000005158
   12          1          -0.000311739   -0.000065377   -0.000000528
   13          6          -0.000051852   -0.000299654    0.000001778
   14          6          -0.000166613   -0.000009272   -0.000000465
   15          6           0.000250409   -0.000490880    0.000003889
   16          1           0.000063310   -0.000107648    0.000000878
   17          1          -0.000105913    0.000216506   -0.000001683
   18          1           0.000208657    0.000240661   -0.000000916
   19          1           0.000104286   -0.000073371    0.000000784
   20          1           0.000036148   -0.000106421    0.000000770
   21          1          -0.000137733    0.000197793   -0.000001680
   22          1           0.000075435   -0.000083316    0.000000772
   23          1           0.000013432   -0.000126798    0.000000849
   24          6          -0.001342339    0.002282626   -0.000018600
   25          7          -0.000317162    0.000539250   -0.000004396
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.002282626 RMS     0.000494917
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.003273753 RMS     0.000360037
 Search for a local minimum.
 Step number   3 out of a maximum of 145
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3
 Trust test= 9.01D-01 RLast= 5.22D-02 DXMaxT set to 4.24D-01
     Eigenvalues ---    0.02070   0.02070   0.02070   0.02084
0.02085
     Eigenvalues ---    0.02088   0.02089   0.02093   0.02097
0.02229
     Eigenvalues ---    0.02231   0.02253   0.02258   0.02349
0.02349
     Eigenvalues ---    0.02380   0.02380   0.02425   0.02429
0.02501
     Eigenvalues ---    0.02504   0.15390   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16051
     Eigenvalues ---    0.21879   0.22000   0.22579   0.22594
0.23100
     Eigenvalues ---    0.24471   0.24560   0.25000   0.25000
0.25000
     Eigenvalues ---    0.25000   0.25238   0.34419   0.36431
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37230   0.37230
0.37230
     Eigenvalues ---    0.37252   0.37386   0.38653   0.39296
0.41636
     Eigenvalues ---    0.42833   0.42950   0.43786   0.44863
0.45327
     Eigenvalues ---    0.45389   0.45632   0.46465   0.47511
0.51569
     Eigenvalues ---    0.51598   0.52934   0.55034
1.344061000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 RFO step:  Lambda=-4.06252792D-05.
 Quartic linear search produced a step of -0.09323.
 Iteration  1 RMS(Cart)=  0.00173779 RMS(Int)=  0.00000064
 Iteration  2 RMS(Cart)=  0.00000130 RMS(Int)=  0.00000010
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000010
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.59209  -0.00036   0.00048  -0.00123  -0.00075
2.59133
    R2        2.69385  -0.00033  -0.00018  -0.00040  -0.00058
2.69327
    R3        2.05375  -0.00014  -0.00009  -0.00015  -0.00024
2.05351
    R4        2.70390  -0.00003  -0.00007   0.00015   0.00008
2.70399
    R5        2.05526  -0.00010  -0.00027   0.00019  -0.00008
2.05518
    R6        2.72475   0.00033  -0.00108   0.00229   0.00121
2.72596
    R7        2.64797  -0.00014   0.00100  -0.00176  -0.00077
2.64721
    R8        2.70037  -0.00035   0.00034  -0.00105  -0.00071
2.69966
    R9        2.67751   0.00105  -0.00008   0.00236   0.00228
2.67979
   R10        2.59565  -0.00025   0.00038  -0.00092  -0.00054
2.59511
   R11        2.05256  -0.00012  -0.00026   0.00013  -0.00013
2.05243
   R12        2.05370  -0.00003  -0.00012   0.00014   0.00002
2.05372
   R13        2.64797  -0.00014   0.00100  -0.00176  -0.00077
2.64721
   R14        2.05634   0.00012  -0.00045   0.00098   0.00053
2.05687
   R15        2.67751   0.00105  -0.00008   0.00236   0.00228
2.67979
   R16        2.69578   0.00327   0.00366   0.00484   0.00850
2.70428
```

This journal is © The Royal Society of Chemistry 2014

R17	2.72475	0.00033	-0.00108	0.00229	0.00121
2.72596					
R18	2.70037	-0.00035	0.00034	-0.00105	-0.00071
2.69966					
R19	2.70390	-0.00003	-0.00007	0.00015	0.00008
2.70399					
R20	2.05526	-0.00010	-0.00027	0.00019	-0.00008
2.05518					
R21	2.59209	-0.00036	0.00048	-0.00123	-0.00075
2.59133					
R22	2.69385	-0.00033	-0.00018	-0.00040	-0.00058
2.69327					
R23	2.05375	-0.00014	-0.00009	-0.00015	-0.00024
2.05351					
R24	2.59565	-0.00025	0.00038	-0.00092	-0.00054
2.59511					
R25	2.05370	-0.00003	-0.00012	0.00014	0.00002
2.05372					
R26	2.05256	-0.00012	-0.00026	0.00013	-0.00013
2.05243					
R27	2.20187	0.00063	-0.00049	0.00110	0.00061
2.20248					
A1	2.09636	-0.00010	0.00005	-0.00064	-0.00059
2.09577					
A2	2.09781	0.00025	-0.00007	0.00154	0.00147
2.09928					
A3	2.08902	-0.00016	0.00001	-0.00090	-0.00088
2.08813					
A4	2.10891	0.00026	0.00007	0.00099	0.00106
2.10998					
A5	2.10421	0.00018	-0.00065	0.00217	0.00152
2.10573					
A6	2.07006	-0.00044	0.00058	-0.00316	-0.00258
2.06748					
A7	2.07628	-0.00023	0.00001	-0.00067	-0.00065
2.07563					
A8	2.12172	0.00040	-0.00016	0.00179	0.00162
2.12335					
A9	2.08518	-0.00017	0.00015	-0.00112	-0.00097
2.08421					
A10	2.06965	-0.00021	0.00015	-0.00101	-0.00086
2.06879					
A11	2.06922	0.00026	-0.00018	0.00130	0.00112
2.07033					
A12	2.14432	-0.00005	0.00003	-0.00028	-0.00026
2.14406					
A13	2.10566	0.00028	0.00014	0.00096	0.00110
2.10676					
A14	2.07792	-0.00019	0.00041	-0.00147	-0.00106
2.07686					
A15	2.09960	-0.00009	-0.00055	0.00051	-0.00003
2.09957					

This journal is © The Royal Society of Chemistry 2014

A16	2.10951	-0.00001	-0.00042	0.00037	-0.00005
2.10945					
A17	2.08545	-0.00010	0.00007	-0.00062	-0.00054
2.08490					
A18	2.08823	0.00012	0.00035	0.00025	0.00060
2.08883					
A19	2.13033	0.00052	-0.00049	0.00242	0.00193
2.13225					
A20	2.07643	-0.00026	0.00025	-0.00121	-0.00096
2.07547					
A21	2.07643	-0.00026	0.00025	-0.00121	-0.00096
2.07547					
A22	2.12725	-0.00071	0.00055	-0.00276	-0.00222
2.12503					
A23	2.07797	0.00035	-0.00027	0.00138	0.00111
2.07908					
A24	2.07797	0.00035	-0.00027	0.00138	0.00111
2.07908					
A25	2.06922	0.00026	-0.00018	0.00130	0.00112
2.07033					
A26	2.14432	-0.00005	0.00003	-0.00028	-0.00026
2.14406					
A27	2.06965	-0.00021	0.00015	-0.00101	-0.00086
2.06879					
A28	2.08518	-0.00017	0.00015	-0.00112	-0.00097
2.08421					
A29	2.12172	0.00040	-0.00016	0.00179	0.00162
2.12335					
A30	2.07628	-0.00023	0.00001	-0.00067	-0.00065
2.07563					
A31	2.07006	-0.00044	0.00058	-0.00316	-0.00258
2.06748					
A32	2.10891	0.00026	0.00007	0.00099	0.00106
2.10998					
A33	2.10421	0.00018	-0.00065	0.00217	0.00152
2.10573					
A34	2.09636	-0.00010	0.00005	-0.00064	-0.00059
2.09577					
A35	2.09781	0.00025	-0.00007	0.00154	0.00147
2.09928					
A36	2.08902	-0.00016	0.00001	-0.00090	-0.00088
2.08813					
A37	2.10951	-0.00001	-0.00042	0.00037	-0.00005
2.10945					
A38	2.08545	-0.00010	0.00007	-0.00062	-0.00054
2.08490					
A39	2.08823	0.00012	0.00035	0.00025	0.00060
2.08883					
A40	2.10566	0.00028	0.00014	0.00096	0.00110
2.10676					
A41	2.07792	-0.00019	0.00041	-0.00147	-0.00106
2.07686					

This journal is © The Royal Society of Chemistry 2014

A42	2.09960	-0.00009	-0.00055	0.00051	-0.00003
2.09957					
A43	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
A44	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D1	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D2	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D3	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D4	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D5	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D6	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D7	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D8	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D9	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D10	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D11	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D12	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D13	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D14	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D15	-3.14159	0.00000	0.00000	0.00000	0.00000	-
3.14159					
D16	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D17	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D18	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D19	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D20	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D21	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D22	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D23	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					

This journal is © The Royal Society of Chemistry 2014

D24	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D25	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D26	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D27	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D28	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D29	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D30	3.14159	0.00000	0.00000	0.00000	0.00000 -
3.14159					
D31	3.14159	0.00000	0.00000	0.00000	0.00000 -
3.14159					
D32	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D33	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D34	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D35	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D36	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D37	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D38	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D39	3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D40	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D41	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D42	-3.14159	0.00000	0.00000	0.00000	0.00000 -
3.14159					
D43	-3.14159	0.00000	0.00000	0.00000	0.00000 -
3.14159					
D44	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D45	-3.14159	0.00000	0.00000	0.00000	0.00000
3.14159					
D46	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D47	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					
D48	3.14159	0.00000	0.00000	0.00000	0.00000 -
3.14159					
D49	0.00000	0.00000	0.00000	0.00000	0.00000
0.00000					

```
   D50        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D51        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D52        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D53        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D54        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D55       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D56        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D57        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D58       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D59       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D60        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D61        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D62        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D63        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D64        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.003274     0.000450     NO
 RMS     Force            0.000360     0.000300     NO
 Maximum Displacement     0.010600     0.001800     NO
 RMS     Displacement     0.001738     0.001200     NO
 Predicted change in Energy=-2.431331D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -5.600502   -0.961912    0.057641
    2          6             0       -4.229359   -0.943288    0.061617
    3          6             0       -3.511420    0.294440    0.055848
    4          6             0       -4.253496    1.531400    0.045724
    5          6             0       -5.680806    1.470879    0.041848
    6          6             0       -6.331465    0.261544    0.047636
    7          6             0       -2.111094    0.332196    0.059790
```

8	6	0	-3.535498	2.754268	0.040050
9	6	0	-2.117807	2.787371	0.044073
10	6	0	-1.397469	1.537627	0.054214
11	6	0	0.033180	1.563456	0.058322
12	1	0	0.568569	0.616843	0.065974
13	6	0	0.715899	2.752682	0.052758
14	6	0	0.001962	3.986150	0.042740
15	6	0	-1.371172	4.005319	0.038516
16	1	0	-1.559341	-0.606009	0.067436
17	1	0	-6.135650	-1.907668	0.062089
18	1	0	-3.662305	-1.871280	0.069244
19	1	0	-6.247027	2.397672	0.034231
20	1	0	-7.417918	0.234977	0.044561
21	1	0	1.802538	2.760677	0.055953
22	1	0	0.553250	4.922717	0.038399
23	1	0	-1.905918	4.950623	0.030875
24	6	0	-4.260919	3.987782	0.029997
25	7	0	-4.851732	4.992408	0.021810

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.371275	0.000000			
3	C	2.437763	1.430888	0.000000		
4	C	2.833932	2.474857	1.442515	0.000000	
5	C	2.434167	2.816965	2.467882	1.428598	0.000000
6	C	1.425220	2.422945	2.820248	2.435260	1.373274
7	C	3.721652	2.472633	1.400841	2.455235	3.746968
8	C	4.251417	3.762158	2.459997	1.418083	2.499888
9	C	5.117272	4.286815	2.856046	2.477627	3.798437
10	C	4.890112	3.764916	2.452408	2.856046	4.283875
11	C	6.173804	4.944999	3.764916	4.286815	5.714760
12	H	6.367886	5.045209	4.092720	4.908068	6.307507
13	C	7.327698	6.173804	4.890112	5.117272	6.523878
14	C	7.474700	6.496444	5.096346	4.912711	6.214535
15	C	6.523878	5.714760	4.283875	3.798437	4.999635
16	H	4.056814	2.691242	2.149780	3.439107	4.615257
17	H	1.086673	2.136346	3.425770	3.920454	3.409087
18	H	2.140956	1.087555	2.171011	3.453735	3.904500
19	H	3.421308	3.903044	3.450739	2.173644	1.086098
20	H	2.176170	3.399339	3.906967	3.419690	2.131905
21	H	8.286294	7.078359	5.858368	6.179545	7.593696
22	H	8.514569	7.568613	6.159772	5.882677	7.125914
23	H	6.971996	6.335417	4.925271	4.147581	5.134054
24	C	5.127837	4.931272	3.768712	2.456443	2.889813
25	N	6.001321	5.968368	4.885539	3.512411	3.617862

		6	7	8	9	10
6	C	0.000000				
7	C	4.220980	0.000000			
8	C	3.745819	2.809938	0.000000		
9	C	4.912711	2.455235	1.418083	0.000000	
10	C	5.096346	1.400841	2.459997	1.442515	0.000000

This journal is © The Royal Society of Chemistry 2014

11	C	6.496444	2.472633	3.762158	2.474857	1.430888
12	H	6.909199	2.694745	4.627378	3.453735	2.171011
13	C	7.474700	3.721651	4.251417	2.833932	2.437763
14	C	7.347449	4.220980	3.745819	2.435260	2.820248
15	C	6.214535	3.746968	2.499888	1.428598	2.467882
16	H	4.850381	1.088447	3.898386	3.439107	2.149780
17	H	2.178080	4.605871	5.338064	6.179545	5.858368
18	H	3.416697	2.694745	4.627378	4.908068	4.092720
19	H	2.137839	4.623072	2.734883	4.147581	4.925271
20	H	1.086782	5.307736	4.628178	5.882677	6.159772
21	H	8.509273	4.605871	5.338064	3.920454	3.425770
22	H	8.314200	5.307736	4.628178	3.419690	3.906967
23	H	6.447728	4.623072	2.734883	2.173644	3.450739
24	C	4.262900	4.240984	1.431045	2.456443	3.768712
25	N	4.956949	5.406488	2.596550	3.512410	4.885539

		11	12	13	14	15
11	C	0.000000				
12	H	1.087555	0.000000			
13	C	1.371275	2.140956	0.000000		
14	C	2.422945	3.416697	1.425220	0.000000	
15	C	2.816965	3.904500	2.434167	1.373274	0.000000
16	H	2.691242	2.454255	4.056814	4.850381	4.615257
17	H	7.078359	7.163778	8.286294	8.509273	7.593696
18	H	5.045209	4.908264	6.367886	6.909199	6.307507
19	H	6.335417	7.044481	6.971996	6.447728	5.134054
20	H	7.568613	7.995639	8.514569	8.314200	7.125914
21	H	2.136346	2.473622	1.086673	2.178080	3.409087
22	H	3.399339	4.305990	2.176170	1.086782	2.131905
23	H	3.903044	4.990588	3.421308	2.137839	1.086098
24	C	4.931272	5.889692	5.127837	4.262900	2.889813
25	N	5.968367	6.966145	6.001321	4.956948	3.617861

		16	17	18	19	20
16	H	0.000000				
17	H	4.757829	0.000000			
18	H	2.454255	2.473622	0.000000		
19	H	5.567549	4.306871	4.990588	0.000000	
20	H	5.918674	2.497087	4.305990	2.459338	0.000000
21	H	4.757829	9.209142	7.163778	8.057776	9.560130
22	H	5.918674	9.560131	7.995639	7.253940	9.247403
23	H	5.567549	8.057776	7.044481	5.036149	7.253940
24	C	5.329431	6.186434	5.889692	2.544227	4.904120
25	N	6.494935	7.018626	6.966146	2.946125	5.405458

		21	22	23	24	25
21	H	0.000000				
22	H	2.497087	0.000000			
23	H	4.306871	2.459338	0.000000		
24	C	6.186434	4.904120	2.544227	0.000000	
25	N	7.018625	5.405457	2.946124	1.165504	0.000000

Stoichiometry C15H9N
Framework group C1[X(C15H9N)]
Deg. of freedom 69
Full point group C1

```
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        3.663849   -1.134900    0.000000
    2          6             0        2.472500   -1.813930    0.000000
    3          6             0        1.226204   -1.110945    0.000000
    4          6             0        1.238814    0.331515    0.000000
    5          6             0        2.499817    1.002903    0.000000
    6          6             0        3.673724    0.290285    0.000000
    7          6             0        0.000000   -1.788277    0.000000
    8          6             0        0.000000    1.021661    0.000000
    9          6             0       -1.238813    0.331515    0.000000
   10          6             0       -1.226204   -1.110945    0.000000
   11          6             0       -2.472499   -1.813931    0.000000
   12          1             0       -2.454132   -2.901331    0.000000
   13          6             0       -3.663849   -1.134901    0.000000
   14          6             0       -3.673724    0.290285    0.000000
   15          6             0       -2.499817    1.002902    0.000000
   16          1             0        0.000000   -2.876725    0.000000
   17          1             0        4.604571   -1.678866    0.000000
   18          1             0        2.454132   -2.901331    0.000000
   19          1             0        2.518074    2.088848    0.000000
   20          1             0        4.623701    0.818148    0.000000
   21          1             0       -4.604571   -1.678867    0.000000
   22          1             0       -4.623701    0.818147    0.000000
   23          1             0       -2.518075    2.088847    0.000000
   24          6             0        0.000000    2.452706    0.000000
   25          7             0       -0.000001    3.618211    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.9800712      0.4486503
0.3077642
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   322 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   322 basis functions,   548 primitive gaussians,   322 cartesian
basis functions
    53 alpha electrons       53 beta electrons
       nuclear repulsion energy       931.1502507686 Hartrees.
 NAtoms=   25 NActive=   25 NUniq=   25 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   322 RedAO= T  NBF=   322
 NBsUse=   315 1.00D-06 NBFU=   315
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -631.795432890     A.U. after   18 cycles
             Convg  =    0.6433D-08             -V/T =  2.0098
             S**2   =   0.0000
 ***** Axes restored to original set *****
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000089515	-0.000063243	0.000000654
2	6	-0.000169851	0.000071919	-0.000000957
3	6	0.000044274	-0.000171136	0.000001219
4	6	-0.000061704	0.000078627	-0.000000679
5	6	0.000149333	0.000018807	0.000000315
6	6	-0.000119604	0.000054072	-0.000000687
7	6	-0.000039218	0.000066678	-0.000000542
8	6	0.000030447	-0.000051800	0.000000423
9	6	-0.000038719	0.000092132	-0.000000710
10	6	0.000128052	-0.000121864	0.000001165
11	6	0.000019694	0.000183387	-0.000001128
12	1	-0.000090470	-0.000009218	-0.000000212
13	6	0.000011763	-0.000108961	0.000000752

```
   14          6           0.000010882    0.000130804   -0.000000821
   15          6          -0.000089024   -0.000121367    0.000000521
   16          1           0.000005659   -0.000009621    0.000000079
   17          1          -0.000008264    0.000072265   -0.000000484
   18          1           0.000052030    0.000074584   -0.000000321
   19          1           0.000001443   -0.000034962    0.000000228
   20          1           0.000039940   -0.000026642    0.000000288
   21          1          -0.000059138    0.000042347   -0.000000449
   22          1           0.000003871   -0.000047854    0.000000319
   23          1           0.000029853   -0.000018253    0.000000205
   24          6          -0.000085921    0.000146169   -0.000001190
   25          7           0.000145159   -0.000246870    0.000002011
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000246870 RMS     0.000073845


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000286392 RMS     0.000048135
 Search for a local minimum.
 Step number   4 out of a maximum of 145
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Update second derivatives using D2CorX and points  1  2  3  4
 Trust test= 9.90D-01 RLast= 1.22D-02 DXMaxT set to 4.24D-01
     Eigenvalues ---    0.02070   0.02070   0.02070   0.02084
0.02085
     Eigenvalues ---    0.02088   0.02089   0.02093   0.02097
0.02229
     Eigenvalues ---    0.02232   0.02253   0.02258   0.02349
0.02349
     Eigenvalues ---    0.02380   0.02380   0.02426   0.02430
0.02501
     Eigenvalues ---    0.02504   0.14491   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16008
0.16017
     Eigenvalues ---    0.21894   0.22000   0.22218   0.22579
0.23000
     Eigenvalues ---    0.24471   0.24514   0.25000   0.25000
0.25000
     Eigenvalues ---    0.25000   0.25341   0.34829   0.36908
0.37230
     Eigenvalues ---    0.37230   0.37230   0.37230   0.37230
0.37230
     Eigenvalues ---    0.37246   0.37474   0.38655   0.40566
0.41961
     Eigenvalues ---    0.42805   0.42947   0.43787   0.44938
0.45328
     Eigenvalues ---    0.45389   0.45632   0.46805   0.48696
0.51548
```

```
     Eigenvalues ---    0.51597   0.52935   0.55609
1.361091000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 RFO step:  Lambda=-8.89866545D-07.
 Quartic linear search produced a step of -0.00410.
 Iteration  1 RMS(Cart)=  0.00040908 RMS(Int)=  0.00000005
 Iteration  2 RMS(Cart)=  0.00000010 RMS(Int)=  0.00000001
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.59133  -0.00005   0.00000  -0.00011  -0.00010
2.59123
    R2        2.69327   0.00000   0.00000  -0.00001   0.00000
2.69327
    R3        2.05351  -0.00006   0.00000  -0.00016  -0.00016
2.05336
    R4        2.70399  -0.00008   0.00000  -0.00017  -0.00017
2.70382
    R5        2.05518  -0.00004   0.00000  -0.00009  -0.00009
2.05509
    R6        2.72596  -0.00001   0.00000   0.00001   0.00001
2.72597
    R7        2.64721   0.00004   0.00000   0.00008   0.00008
2.64729
    R8        2.69966  -0.00011   0.00000  -0.00024  -0.00024
2.69942
```

This journal is © The Royal Society of Chemistry 2014

R9	2.67979	-0.00014	-0.00001	-0.00026	-0.00027
2.67952					
R10	2.59511	-0.00002	0.00000	-0.00005	-0.00004
2.59507					
R11	2.05243	-0.00003	0.00000	-0.00008	-0.00008
2.05235					
R12	2.05372	-0.00004	0.00000	-0.00010	-0.00010
2.05362					
R13	2.64721	0.00004	0.00000	0.00008	0.00008
2.64729					
R14	2.05687	0.00001	0.00000	0.00005	0.00005
2.05692					
R15	2.67979	-0.00014	-0.00001	-0.00026	-0.00027
2.67952					
R16	2.70428	-0.00012	-0.00003	-0.00021	-0.00025
2.70404					
R17	2.72596	-0.00001	0.00000	0.00001	0.00001
2.72597					
R18	2.69966	-0.00011	0.00000	-0.00024	-0.00024
2.69942					
R19	2.70399	-0.00008	0.00000	-0.00017	-0.00017
2.70382					
R20	2.05518	-0.00004	0.00000	-0.00009	-0.00009
2.05509					
R21	2.59133	-0.00005	0.00000	-0.00011	-0.00010
2.59123					
R22	2.69327	0.00000	0.00000	-0.00001	0.00000
2.69327					
R23	2.05351	-0.00006	0.00000	-0.00016	-0.00016
2.05336					
R24	2.59511	-0.00002	0.00000	-0.00005	-0.00004
2.59507					
R25	2.05372	-0.00004	0.00000	-0.00010	-0.00010
2.05362					
R26	2.05243	-0.00003	0.00000	-0.00008	-0.00008
2.05235					
R27	2.20248	-0.00029	0.00000	-0.00019	-0.00019
2.20230					
A1	2.09577	0.00000	0.00000	0.00001	0.00001
2.09578					
A2	2.09928	0.00004	-0.00001	0.00031	0.00030
2.09958					
A3	2.08813	-0.00005	0.00000	-0.00031	-0.00031
2.08783					
A4	2.10998	0.00005	0.00000	0.00026	0.00026
2.11023					
A5	2.10573	0.00006	-0.00001	0.00047	0.00046
2.10619					
A6	2.06748	-0.00011	0.00001	-0.00073	-0.00072
2.06676					
A7	2.07563	-0.00007	0.00000	-0.00033	-0.00033
2.07530					

This journal is © The Royal Society of Chemistry 2014

A8	2.12335	0.00011	-0.00001	0.00050	0.00049
2.12384					
A9	2.08421	-0.00004	0.00000	-0.00017	-0.00016
2.08404					
A10	2.06879	0.00004	0.00000	0.00015	0.00016
2.06894					
A11	2.07033	0.00001	0.00000	0.00002	0.00001
2.07035					
A12	2.14406	-0.00005	0.00000	-0.00017	-0.00017
2.14390					
A13	2.10676	0.00002	0.00000	0.00015	0.00014
2.10690					
A14	2.07686	0.00001	0.00000	0.00002	0.00002
2.07688					
A15	2.09957	-0.00003	0.00000	-0.00016	-0.00016
2.09941					
A16	2.10945	-0.00006	0.00000	-0.00024	-0.00024
2.10921					
A17	2.08490	0.00000	0.00000	-0.00007	-0.00007
2.08483					
A18	2.08883	0.00006	0.00000	0.00031	0.00031
2.08914					
A19	2.13225	0.00000	-0.00001	0.00013	0.00013
2.13238					
A20	2.07547	0.00000	0.00000	-0.00007	-0.00006
2.07540					
A21	2.07547	0.00000	0.00000	-0.00007	-0.00006
2.07540					
A22	2.12503	0.00007	0.00001	0.00017	0.00018
2.12521					
A23	2.07908	-0.00004	0.00000	-0.00008	-0.00009
2.07899					
A24	2.07908	-0.00004	0.00000	-0.00008	-0.00009
2.07899					
A25	2.07033	0.00001	0.00000	0.00002	0.00001
2.07035					
A26	2.14406	-0.00005	0.00000	-0.00017	-0.00017
2.14390					
A27	2.06879	0.00004	0.00000	0.00015	0.00016
2.06894					
A28	2.08421	-0.00004	0.00000	-0.00017	-0.00016
2.08404					
A29	2.12335	0.00011	-0.00001	0.00050	0.00049
2.12384					
A30	2.07563	-0.00007	0.00000	-0.00033	-0.00033
2.07530					
A31	2.06748	-0.00011	0.00001	-0.00073	-0.00072
2.06676					
A32	2.10998	0.00005	0.00000	0.00026	0.00026
2.11023					
A33	2.10573	0.00006	-0.00001	0.00047	0.00046
2.10619					

This journal is © The Royal Society of Chemistry 2014

```
   A34        2.09577   0.00000   0.00000   0.00001   0.00001
2.09578
   A35        2.09928   0.00004  -0.00001   0.00031   0.00030
2.09958
   A36        2.08813  -0.00005   0.00000  -0.00031  -0.00031
2.08783
   A37        2.10945  -0.00006   0.00000  -0.00024  -0.00024
2.10921
   A38        2.08490   0.00000   0.00000  -0.00007  -0.00007
2.08483
   A39        2.08883   0.00006   0.00000   0.00031   0.00031
2.08914
   A40        2.10676   0.00002   0.00000   0.00015   0.00014
2.10690
   A41        2.07686   0.00001   0.00000   0.00002   0.00002
2.07688
   A42        2.09957  -0.00003   0.00000  -0.00016  -0.00016
2.09941
   A43        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   A44        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
    D1        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D2       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
    D3        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
    D4        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D5        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D6        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
    D7       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
    D8        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
    D9        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D10        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D11        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D12        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D13        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D14       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D15       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
```

This journal is © The Royal Society of Chemistry 2014

```
   D16        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D17        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D18        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D19        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D20        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D21        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D22        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D23        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D24        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D25        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D26        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D27        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D28        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D29        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D30       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D31       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D32        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D33        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D34        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D35        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D36        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D37        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D38        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D39        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D40        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D41        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
```

This journal is © The Royal Society of Chemistry 2014

```
   D42       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D43       -3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D44        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D45        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D46        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D47        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D48       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D49        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D50        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D51        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D52        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D53        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D54       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D55       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D56        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D57        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D58        3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D59        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D60        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D61        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
   D62       -3.14159   0.00000   0.00000   0.00000   0.00000
3.14159
   D63        3.14159   0.00000   0.00000   0.00000   0.00000  -
3.14159
   D64        0.00000   0.00000   0.00000   0.00000   0.00000
0.00000
         Item               Value     Threshold  Converged?
 Maximum Force            0.000286     0.000450     YES
 RMS     Force            0.000048     0.000300     YES
 Maximum Displacement     0.001681     0.001800     YES
 RMS     Displacement     0.000409     0.001200     YES
 Predicted change in Energy=-4.454110D-07
```

This journal is © The Royal Society of Chemistry 2014

Optimization completed.
-- Stationary point found.

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.3713	-DE/DX = 0.0
R2	R(1,6)	1.4252	-DE/DX = 0.0
R3	R(1,17)	1.0867	-DE/DX = -0.0001
R4	R(2,3)	1.4309	-DE/DX = -0.0001
R5	R(2,18)	1.0876	-DE/DX = 0.0
R6	R(3,4)	1.4425	-DE/DX = 0.0
R7	R(3,7)	1.4008	-DE/DX = 0.0
R8	R(4,5)	1.4286	-DE/DX = -0.0001
R9	R(4,8)	1.4181	-DE/DX = -0.0001
R10	R(5,6)	1.3733	-DE/DX = 0.0
R11	R(5,19)	1.0861	-DE/DX = 0.0
R12	R(6,20)	1.0868	-DE/DX = 0.0
R13	R(7,10)	1.4008	-DE/DX = 0.0
R14	R(7,16)	1.0884	-DE/DX = 0.0
R15	R(8,9)	1.4181	-DE/DX = -0.0001
R16	R(8,24)	1.431	-DE/DX = -0.0001
R17	R(9,10)	1.4425	-DE/DX = 0.0
R18	R(9,15)	1.4286	-DE/DX = -0.0001
R19	R(10,11)	1.4309	-DE/DX = -0.0001
R20	R(11,12)	1.0876	-DE/DX = 0.0

This journal is © The Royal Society of Chemistry 2014

```
 ! R21   R(11,13)                1.3713         -DE/DX =    0.0
!
 ! R22   R(13,14)                1.4252         -DE/DX =    0.0
!
 ! R23   R(13,21)                1.0867         -DE/DX =   -0.0001
!
 ! R24   R(14,15)                1.3733         -DE/DX =    0.0
!
 ! R25   R(14,22)                1.0868         -DE/DX =    0.0
!
 ! R26   R(15,23)                1.0861         -DE/DX =    0.0
!
 ! R27   R(24,25)                1.1655         -DE/DX =   -0.0003
!
 ! A1    A(2,1,6)               120.0787        -DE/DX =    0.0
!
 ! A2    A(2,1,17)              120.2799        -DE/DX =    0.0
!
 ! A3    A(6,1,17)              119.6413        -DE/DX =    0.0
!
 ! A4    A(1,2,3)               120.8927        -DE/DX =    0.0001
!
 ! A5    A(1,2,18)              120.6494        -DE/DX =    0.0001
!
 ! A6    A(3,2,18)              118.4579        -DE/DX =   -0.0001
!
 ! A7    A(2,3,4)               118.9248        -DE/DX =   -0.0001
!
 ! A8    A(2,3,7)               121.659         -DE/DX =    0.0001
!
 ! A9    A(4,3,7)               119.4163        -DE/DX =    0.0
!
 ! A10   A(3,4,5)               118.5327        -DE/DX =    0.0
!
 ! A11   A(3,4,8)               118.6214        -DE/DX =    0.0
!
 ! A12   A(5,4,8)               122.8458        -DE/DX =   -0.0001
!
 ! A13   A(4,5,6)               120.7084        -DE/DX =    0.0
!
 ! A14   A(4,5,19)              118.9951        -DE/DX =    0.0
!
 ! A15   A(6,5,19)              120.2966        -DE/DX =    0.0
!
 ! A16   A(1,6,5)               120.8627        -DE/DX =   -0.0001
!
 ! A17   A(1,6,20)              119.4561        -DE/DX =    0.0
!
 ! A18   A(5,6,20)              119.6811        -DE/DX =    0.0001
!
 ! A19   A(3,7,10)              122.1691        -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A20   A(3,7,16)             118.9154         -DE/DX =    0.0
!
 ! A21   A(10,7,16)            118.9154         -DE/DX =    0.0
!
 ! A22   A(4,8,9)              121.7554         -DE/DX =    0.0001
!
 ! A23   A(4,8,24)             119.1223         -DE/DX =    0.0
!
 ! A24   A(9,8,24)             119.1223         -DE/DX =    0.0
!
 ! A25   A(8,9,10)             118.6214         -DE/DX =    0.0
!
 ! A26   A(8,9,15)             122.8458         -DE/DX =   -0.0001
!
 ! A27   A(10,9,15)            118.5327         -DE/DX =    0.0
!
 ! A28   A(7,10,9)             119.4163         -DE/DX =    0.0
!
 ! A29   A(7,10,11)            121.6589         -DE/DX =    0.0001
!
 ! A30   A(9,10,11)            118.9248         -DE/DX =   -0.0001
!
 ! A31   A(10,11,12)           118.4579         -DE/DX =   -0.0001
!
 ! A32   A(10,11,13)           120.8927         -DE/DX =    0.0001
!
 ! A33   A(12,11,13)           120.6494         -DE/DX =    0.0001
!
 ! A34   A(11,13,14)           120.0787         -DE/DX =    0.0
!
 ! A35   A(11,13,21)           120.2799         -DE/DX =    0.0
!
 ! A36   A(14,13,21)           119.6413         -DE/DX =    0.0
!
 ! A37   A(13,14,15)           120.8627         -DE/DX =   -0.0001
!
 ! A38   A(13,14,22)           119.4561         -DE/DX =    0.0
!
 ! A39   A(15,14,22)           119.6811         -DE/DX =    0.0001
!
 ! A40   A(9,15,14)            120.7084         -DE/DX =    0.0
!
 ! A41   A(9,15,23)            118.9951         -DE/DX =    0.0
!
 ! A42   A(14,15,23)           120.2966         -DE/DX =    0.0
!
 ! A43   L(8,24,25,9,-1)       180.0            -DE/DX =    0.0
!
 ! A44   L(8,24,25,9,-2)       180.0            -DE/DX =    0.0
!
 ! D1    D(6,1,2,3)              0.0            -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D2    D(6,1,2,18)           180.0            -DE/DX =    0.0
!
 ! D3    D(17,1,2,3)           180.0            -DE/DX =    0.0
!
 ! D4    D(17,1,2,18)            0.0            -DE/DX =    0.0
!
 ! D5    D(2,1,6,5)              0.0            -DE/DX =    0.0
!
 ! D6    D(2,1,6,20)           180.0            -DE/DX =    0.0
!
 ! D7    D(17,1,6,5)          -180.0            -DE/DX =    0.0
!
 ! D8    D(17,1,6,20)            0.0            -DE/DX =    0.0
!
 ! D9    D(1,2,3,4)              0.0            -DE/DX =    0.0
!
 ! D10   D(1,2,3,7)            180.0            -DE/DX =    0.0
!
 ! D11   D(18,2,3,4)           180.0            -DE/DX =    0.0
!
 ! D12   D(18,2,3,7)             0.0            -DE/DX =    0.0
!
 ! D13   D(2,3,4,5)              0.0            -DE/DX =    0.0
!
 ! D14   D(2,3,4,8)           -180.0            -DE/DX =    0.0
!
 ! D15   D(7,3,4,5)           -180.0            -DE/DX =    0.0
!
 ! D16   D(7,3,4,8)              0.0            -DE/DX =    0.0
!
 ! D17   D(2,3,7,10)           180.0            -DE/DX =    0.0
!
 ! D18   D(2,3,7,16)             0.0            -DE/DX =    0.0
!
 ! D19   D(4,3,7,10)             0.0            -DE/DX =    0.0
!
 ! D20   D(4,3,7,16)           180.0            -DE/DX =    0.0
!
 ! D21   D(3,4,5,6)              0.0            -DE/DX =    0.0
!
 ! D22   D(3,4,5,19)           180.0            -DE/DX =    0.0
!
 ! D23   D(8,4,5,6)            180.0            -DE/DX =    0.0
!
 ! D24   D(8,4,5,19)             0.0            -DE/DX =    0.0
!
 ! D25   D(3,4,8,9)              0.0            -DE/DX =    0.0
!
 ! D26   D(3,4,8,24)           180.0            -DE/DX =    0.0
!
 ! D27   D(5,4,8,9)            180.0            -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D28   D(5,4,8,24)             0.0             -DE/DX =    0.0
!
 ! D29   D(4,5,6,1)              0.0             -DE/DX =    0.0
!
 ! D30   D(4,5,6,20)           180.0             -DE/DX =    0.0
!
 ! D31   D(19,5,6,1)           180.0             -DE/DX =    0.0
!
 ! D32   D(19,5,6,20)            0.0             -DE/DX =    0.0
!
 ! D33   D(3,7,10,9)             0.0             -DE/DX =    0.0
!
 ! D34   D(3,7,10,11)         -180.0             -DE/DX =    0.0
!
 ! D35   D(16,7,10,9)          180.0             -DE/DX =    0.0
!
 ! D36   D(16,7,10,11)           0.0             -DE/DX =    0.0
!
 ! D37   D(4,8,9,10)             0.0             -DE/DX =    0.0
!
 ! D38   D(4,8,9,15)           180.0             -DE/DX =    0.0
!
 ! D39   D(24,8,9,10)          180.0             -DE/DX =    0.0
!
 ! D40   D(24,8,9,15)            0.0             -DE/DX =    0.0
!
 ! D41   D(8,9,10,7)             0.0             -DE/DX =    0.0
!
 ! D42   D(8,9,10,11)          180.0             -DE/DX =    0.0
!
 ! D43   D(15,9,10,7)         -180.0             -DE/DX =    0.0
!
 ! D44   D(15,9,10,11)           0.0             -DE/DX =    0.0
!
 ! D45   D(8,9,15,14)         -180.0             -DE/DX =    0.0
!
 ! D46   D(8,9,15,23)            0.0             -DE/DX =    0.0
!
 ! D47   D(10,9,15,14)           0.0             -DE/DX =    0.0
!
 ! D48   D(10,9,15,23)         180.0             -DE/DX =    0.0
!
 ! D49   D(7,10,11,12)           0.0             -DE/DX =    0.0
!
 ! D50   D(7,10,11,13)         180.0             -DE/DX =    0.0
!
 ! D51   D(9,10,11,12)         180.0             -DE/DX =    0.0
!
 ! D52   D(9,10,11,13)           0.0             -DE/DX =    0.0
!
 ! D53   D(10,11,13,14)          0.0             -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D54   D(10,11,13,21)        180.0            -DE/DX =    0.0
!
 ! D55   D(12,11,13,14)        180.0            -DE/DX =    0.0
!
 ! D56   D(12,11,13,21)          0.0            -DE/DX =    0.0
!
 ! D57   D(11,13,14,15)          0.0            -DE/DX =    0.0
!
 ! D58   D(11,13,14,22)        180.0            -DE/DX =    0.0
!
 ! D59   D(21,13,14,15)       -180.0            -DE/DX =    0.0
!
 ! D60   D(21,13,14,22)          0.0            -DE/DX =    0.0
!
 ! D61   D(13,14,15,9)           0.0            -DE/DX =    0.0
!
 ! D62   D(13,14,15,23)        180.0            -DE/DX =    0.0
!
 ! D63   D(22,14,15,9)        -180.0            -DE/DX =    0.0
!
 ! D64   D(22,14,15,23)          0.0            -DE/DX =    0.0
!
 ---------------------------------------------------------------------
-----------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -5.600502   -0.961912    0.057641
    2          6             0       -4.229359   -0.943288    0.061617
    3          6             0       -3.511420    0.294440    0.055848
    4          6             0       -4.253496    1.531400    0.045724
    5          6             0       -5.680806    1.470879    0.041848
    6          6             0       -6.331465    0.261544    0.047636
    7          6             0       -2.111094    0.332196    0.059790
    8          6             0       -3.535498    2.754268    0.040050
    9          6             0       -2.117807    2.787371    0.044073
   10          6             0       -1.397469    1.537627    0.054214
   11          6             0        0.033180    1.563456    0.058322
   12          1             0        0.568569    0.616843    0.065974
   13          6             0        0.715899    2.752682    0.052758
   14          6             0        0.001962    3.986150    0.042740
   15          6             0       -1.371172    4.005319    0.038516
   16          1             0       -1.559341   -0.606009    0.067436
   17          1             0       -6.135650   -1.907668    0.062089
   18          1             0       -3.662305   -1.871280    0.069244
   19          1             0       -6.247027    2.397672    0.034231
```

20	1	0	-7.417918	0.234977	0.044561
21	1	0	1.802538	2.760677	0.055953
22	1	0	0.553250	4.922717	0.038399
23	1	0	-1.905918	4.950623	0.030875
24	6	0	-4.260919	3.987782	0.029997
25	7	0	-4.851732	4.992408	0.021810

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.371275	0.000000			
3	C	2.437763	1.430888	0.000000		
4	C	2.833932	2.474857	1.442515	0.000000	
5	C	2.434167	2.816965	2.467882	1.428598	0.000000
6	C	1.425220	2.422945	2.820248	2.435260	1.373274
7	C	3.721652	2.472633	1.400841	2.455235	3.746968
8	C	4.251417	3.762158	2.459997	1.418083	2.499888
9	C	5.117272	4.286815	2.856046	2.477627	3.798437
10	C	4.890112	3.764916	2.452408	2.856046	4.283875
11	C	6.173804	4.944999	3.764916	4.286815	5.714760
12	H	6.367886	5.045209	4.092720	4.908068	6.307507
13	C	7.327698	6.173804	4.890112	5.117272	6.523878
14	C	7.474700	6.496444	5.096346	4.912711	6.214535
15	C	6.523878	5.714760	4.283875	3.798437	4.999635
16	H	4.056814	2.691242	2.149780	3.439107	4.615257
17	H	1.086673	2.136346	3.425770	3.920454	3.409087
18	H	2.140956	1.087555	2.171011	3.453735	3.904500
19	H	3.421308	3.903044	3.450739	2.173644	1.086098
20	H	2.176170	3.399339	3.906967	3.419690	2.131905
21	H	8.286294	7.078359	5.858368	6.179545	7.593696
22	H	8.514569	7.568613	6.159772	5.882677	7.125914
23	H	6.971996	6.335417	4.925271	4.147581	5.134054
24	C	5.127837	4.931272	3.768712	2.456443	2.889813
25	N	6.001321	5.968368	4.885539	3.512411	3.617862

		6	7	8	9	10
6	C	0.000000				
7	C	4.220980	0.000000			
8	C	3.745819	2.809938	0.000000		
9	C	4.912711	2.455235	1.418083	0.000000	
10	C	5.096346	1.400841	2.459997	1.442515	0.000000
11	C	6.496444	2.472633	3.762158	2.474857	1.430888
12	H	6.909199	2.694745	4.627378	3.453735	2.171011
13	C	7.474700	3.721651	4.251417	2.833932	2.437763
14	C	7.347449	4.220980	3.745819	2.435260	2.820248
15	C	6.214535	3.746968	2.499888	1.428598	2.467882
16	H	4.850381	1.088447	3.898386	3.439107	2.149780
17	H	2.178080	4.605871	5.338064	6.179545	5.858368
18	H	3.416697	2.694745	4.627378	4.908068	4.092720
19	H	2.137839	4.623072	2.734883	4.147581	4.925271
20	H	1.086782	5.307736	4.628178	5.882677	6.159772
21	H	8.509273	4.605871	5.338064	3.920454	3.425770
22	H	8.314200	5.307736	4.628178	3.419690	3.906967

This journal is © The Royal Society of Chemistry 2014

23	H	6.447728	4.623072	2.734883	2.173644	3.450739
24	C	4.262900	4.240984	1.431045	2.456443	3.768712
25	N	4.956949	5.406488	2.596550	3.512410	4.885539

		11	12	13	14	15
11	C	0.000000				
12	H	1.087555	0.000000			
13	C	1.371275	2.140956	0.000000		
14	C	2.422945	3.416697	1.425220	0.000000	
15	C	2.816965	3.904500	2.434167	1.373274	0.000000
16	H	2.691242	2.454255	4.056814	4.850381	4.615257
17	H	7.078359	7.163778	8.286294	8.509273	7.593696
18	H	5.045209	4.908264	6.367886	6.909199	6.307507
19	H	6.335417	7.044481	6.971996	6.447728	5.134054
20	H	7.568613	7.995639	8.514569	8.314200	7.125914
21	H	2.136346	2.473622	1.086673	2.178080	3.409087
22	H	3.399339	4.305990	2.176170	1.086782	2.131905
23	H	3.903044	4.990588	3.421308	2.137839	1.086098
24	C	4.931272	5.889692	5.127837	4.262900	2.889813
25	N	5.968367	6.966145	6.001321	4.956948	3.617861

		16	17	18	19	20
16	H	0.000000				
17	H	4.757829	0.000000			
18	H	2.454255	2.473622	0.000000		
19	H	5.567549	4.306871	4.990588	0.000000	
20	H	5.918674	2.497087	4.305990	2.459338	0.000000
21	H	4.757829	9.209142	7.163778	8.057776	9.560130
22	H	5.918674	9.560131	7.995639	7.253940	9.247403
23	H	5.567549	8.057776	7.044481	5.036149	7.253940
24	C	5.329431	6.186434	5.889692	2.544227	4.904120
25	N	6.494935	7.018626	6.966146	2.946125	5.405458

		21	22	23	24	25
21	H	0.000000				
22	H	2.497087	0.000000			
23	H	4.306871	2.459338	0.000000		
24	C	6.186434	4.904120	2.544227	0.000000	
25	N	7.018625	5.405457	2.946124	1.165504	0.000000

Stoichiometry C15H9N
Framework group C1[X(C15H9N)]
Deg. of freedom 69
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.663849	-1.134900	0.000000
2	6	0	2.472500	-1.813930	0.000000
3	6	0	1.226204	-1.110945	0.000000
4	6	0	1.238814	0.331515	0.000000
5	6	0	2.499817	1.002903	0.000000

6	6	0	3.673724	0.290285	0.000000
7	6	0	0.000000	-1.788277	0.000000
8	6	0	0.000000	1.021661	0.000000
9	6	0	-1.238813	0.331515	0.000000
10	6	0	-1.226204	-1.110945	0.000000
11	6	0	-2.472499	-1.813931	0.000000
12	1	0	-2.454132	-2.901331	0.000000
13	6	0	-3.663849	-1.134901	0.000000
14	6	0	-3.673724	0.290285	0.000000
15	6	0	-2.499817	1.002902	0.000000
16	1	0	0.000000	-2.876725	0.000000
17	1	0	4.604571	-1.678866	0.000000
18	1	0	2.454132	-2.901331	0.000000
19	1	0	2.518074	2.088848	0.000000
20	1	0	4.623701	0.818148	0.000000
21	1	0	-4.604571	-1.678867	0.000000
22	1	0	-4.623701	0.818147	0.000000
23	1	0	-2.518075	2.088847	0.000000
24	6	0	0.000000	2.452706	0.000000
25	7	0	-0.000001	3.618211	0.000000

Rotational constants (GHZ): 0.9800712 0.4486503 0.3077642

****

Population analysis using the SCF density.

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -14.34602 -10.24494 -10.23772 -10.23390 -
10.23388
 Alpha  occ. eigenvalues --  -10.22733 -10.22729 -10.22425 -10.21641 -
10.21641
 Alpha  occ. eigenvalues --  -10.21570 -10.21570 -10.21440 -10.21440 -
10.21241
 Alpha  occ. eigenvalues --  -10.21241  -0.92110  -0.90180  -0.87354
-0.82751
 Alpha  occ. eigenvalues --   -0.81599  -0.77498  -0.76385  -0.73499
-0.67588
 Alpha  occ. eigenvalues --   -0.64733  -0.64193  -0.61407  -0.56979
-0.54819
 Alpha  occ. eigenvalues --   -0.54444  -0.50053  -0.48927  -0.48384
-0.47198
 Alpha  occ. eigenvalues --   -0.44942  -0.44799  -0.43328  -0.43202
-0.41869
 Alpha  occ. eigenvalues --   -0.39994  -0.38390  -0.37423  -0.37178
-0.37012
 Alpha  occ. eigenvalues --   -0.36544  -0.35371  -0.33767  -0.32480
-0.30802
 Alpha  occ. eigenvalues --   -0.27915  -0.26558  -0.22062
 Alpha virt. eigenvalues --   -0.09855  -0.04109  -0.02286  -0.01979
-0.00249
 Alpha virt. eigenvalues --    0.00411   0.01197   0.01719   0.02599
0.02702
 Alpha virt. eigenvalues --    0.02910   0.03985   0.04709   0.04840
0.04871
 Alpha virt. eigenvalues --    0.05964   0.06320   0.06907   0.07017
0.07435
 Alpha virt. eigenvalues --    0.08407   0.09104   0.09541   0.09832
0.11091
 Alpha virt. eigenvalues --    0.11123   0.11391   0.11622   0.12599
0.12875
 Alpha virt. eigenvalues --    0.13549   0.13582   0.14101   0.14447
0.14821
 Alpha virt. eigenvalues --    0.16277   0.16909   0.17256   0.17437
0.17504
 Alpha virt. eigenvalues --    0.17544   0.17775   0.18751   0.19034
0.19248
 Alpha virt. eigenvalues --    0.19592   0.20035   0.20510   0.20887
0.21703
 Alpha virt. eigenvalues --    0.21963   0.22249   0.22901   0.22975
0.23903
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.23938   0.24955   0.24987   0.25356
0.25568
 Alpha virt. eigenvalues --    0.26056   0.26380   0.26997   0.27269
0.27342
 Alpha virt. eigenvalues --    0.27430   0.28083   0.28817   0.28854
0.29915
 Alpha virt. eigenvalues --    0.30092   0.30526   0.30567   0.31375
0.32776
 Alpha virt. eigenvalues --    0.32938   0.33487   0.35169   0.36638
0.36855
 Alpha virt. eigenvalues --    0.37662   0.38208   0.40680   0.41418
0.44415
 Alpha virt. eigenvalues --    0.46452   0.47634   0.49087   0.55308
0.57127
 Alpha virt. eigenvalues --    0.60779   0.63342   0.63588   0.64014
0.65462
 Alpha virt. eigenvalues --    0.65871   0.67542   0.69643   0.69870
0.70314
 Alpha virt. eigenvalues --    0.70790   0.70804   0.70851   0.71723
0.72149
 Alpha virt. eigenvalues --    0.72902   0.73091   0.74735   0.75702
0.76310
 Alpha virt. eigenvalues --    0.76415   0.77038   0.77537   0.78475
0.78874
 Alpha virt. eigenvalues --    0.79468   0.79623   0.81543   0.84211
0.84511
 Alpha virt. eigenvalues --    0.86958   0.88014   0.88418   0.89017
0.90817
 Alpha virt. eigenvalues --    0.91236   0.91409   0.93956   0.95182
0.95707
 Alpha virt. eigenvalues --    0.99398   1.00072   1.02796   1.03280
1.03981
 Alpha virt. eigenvalues --    1.06096   1.07290   1.07762   1.09843
1.11324
 Alpha virt. eigenvalues --    1.11818   1.11897   1.14743   1.15782
1.17393
 Alpha virt. eigenvalues --    1.17859   1.18475   1.19880   1.20467
1.22369
 Alpha virt. eigenvalues --    1.23014   1.24096   1.24528   1.25478
1.31286
 Alpha virt. eigenvalues --    1.31794   1.32242   1.33962   1.35279
1.38541
 Alpha virt. eigenvalues --    1.39218   1.41866   1.42213   1.44845
1.45901
 Alpha virt. eigenvalues --    1.46373   1.46852   1.47097   1.47745
1.47991
 Alpha virt. eigenvalues --    1.52095   1.52167   1.53555   1.56317
1.57040
 Alpha virt. eigenvalues --    1.64895   1.67621   1.72600   1.75501
1.78900
 Alpha virt. eigenvalues --    1.80021   1.81279   1.82325   1.87588
1.87803
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    1.88433   1.90691   1.91021   1.93647
1.94128
 Alpha virt. eigenvalues --    1.94385   1.94967   1.95331   1.96725
1.98247
 Alpha virt. eigenvalues --    2.00305   2.02972   2.02982   2.04170
2.05504
 Alpha virt. eigenvalues --    2.10255   2.14519   2.14987   2.16360
2.18853
 Alpha virt. eigenvalues --    2.19890   2.20719   2.22389   2.24270
2.25476
 Alpha virt. eigenvalues --    2.27665   2.28747   2.32109   2.32433
2.32446
 Alpha virt. eigenvalues --    2.35629   2.37496   2.39872   2.44264
2.47347
 Alpha virt. eigenvalues --    2.55601   2.60626   2.61004   2.61053
2.63861
 Alpha virt. eigenvalues --    2.66601   2.67702   2.70722   2.71787
2.72204
 Alpha virt. eigenvalues --    2.75479   2.79545   2.81373   2.83225
2.84296
 Alpha virt. eigenvalues --    2.84566   2.89586   2.93237   2.99308
3.06381
 Alpha virt. eigenvalues --    3.10257   3.20129   3.24702   3.33208
3.44411
 Alpha virt. eigenvalues --    3.51693   4.20425   4.22592   4.23746
4.25920
 Alpha virt. eigenvalues --    4.29238   4.30823   4.31082   4.31862
4.36179
 Alpha virt. eigenvalues --    4.40542   4.41624   4.44817   4.48389
4.63646
 Alpha virt. eigenvalues --    4.66224   4.91118
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C    5.876661   0.322715  -0.475083   0.175010  -0.727730
0.933829
     2  C    0.322715   6.908713  -0.238428  -0.882641   1.420327  -
1.118370
     3  C   -0.475083  -0.238428   7.831739   0.271124   0.841144  -
0.335543
     4  C    0.175010  -0.882641   0.271124   9.122115  -3.039735
0.867293
     5  C   -0.727730   1.420327   0.841144  -3.039735  11.433280  -
2.832654
     6  C    0.933829  -1.118370  -0.335543   0.867293  -2.832654
8.296963
     7  C    0.014864  -0.048585   0.428599  -0.982636   0.755107  -
0.472297
     8  C    0.017995  -0.314401  -0.329504   1.435129  -1.246587
0.425831
     9  C   -0.015169  -0.051095  -0.657124   0.050974  -0.348825
0.282555
```

This journal is © The Royal Society of Chemistry 2014

10	C	0.004460	0.187162	-0.738693	-0.657125	-0.127752	0.016772
11	C	-0.031183	-0.188935	0.187162	-0.051095	-0.128289	0.061249
12	H	0.000784	0.004849	-0.006213	0.000376	0.000034	-0.000030
13	C	0.016036	-0.031183	0.004460	-0.015169	-0.041021	0.003230
14	C	0.003230	0.061249	0.016772	0.282554	0.062080	-0.062553
15	C	-0.041021	-0.128289	-0.127752	-0.348825	-0.141943	0.062080
16	H	-0.000004	0.005538	-0.050920	0.008077	0.002725	0.001744
17	H	0.294864	-0.016462	0.016756	0.020403	-0.008304	0.000929
18	H	0.014153	0.270320	-0.050388	0.057945	-0.031971	0.007803
19	H	0.013738	-0.017023	0.026335	-0.074608	0.294304	0.027589
20	H	-0.016741	0.008844	0.009067	-0.006211	0.005474	0.304377
21	H	-0.000001	0.000054	-0.001721	0.000607	0.000002	-0.000005
22	H	0.000001	0.000012	0.001120	-0.000744	-0.000131	-0.000003
23	H	0.000026	-0.000507	-0.002806	0.000975	0.005571	0.000981
24	C	-0.001811	-0.118080	-1.094106	-0.885542	0.380119	0.044458
25	N	-0.000499	0.004335	0.064016	0.022636	-0.002311	0.030450

		7	8	9	10	11	12
1	C	0.014864	0.017995	-0.015169	0.004460	-0.031183	0.000784
2	C	-0.048585	-0.314401	-0.051095	0.187162	-0.188935	0.004849
3	C	0.428599	-0.329504	-0.657124	-0.738693	0.187162	-0.006213
4	C	-0.982636	1.435129	0.050974	-0.657125	-0.051095	0.000376
5	C	0.755107	-1.246587	-0.348825	-0.127752	-0.128289	0.000034
6	C	-0.472297	0.425831	0.282555	0.016772	0.061249	-0.000030
7	C	6.898363	-0.483457	-0.982635	0.428599	-0.048585	0.004479
8	C	-0.483457	7.047430	1.435129	-0.329504	-0.314401	0.006583
9	C	-0.982635	1.435129	9.122115	0.271124	-0.882640	0.057945

This journal is © The Royal Society of Chemistry 2014

10	C	0.428599	-0.329504	0.271124	7.831738	-0.238427	-0.050388
11	C	-0.048585	-0.314401	-0.882640	-0.238427	6.908714	0.270320
12	H	0.004479	0.006583	0.057945	-0.050388	0.270320	0.534371
13	C	0.014864	0.017995	0.175010	-0.475082	0.322714	0.014153
14	C	-0.472297	0.425832	0.867294	-0.335544	-1.118370	0.007803
15	C	0.755107	-1.246587	-3.039736	0.841146	1.420326	-0.031971
16	H	0.339799	-0.001407	0.008077	-0.050920	0.005539	0.004147
17	H	-0.011626	0.001747	0.000607	-0.001721	0.000054	0.000000
18	H	0.004478	0.006583	0.000376	-0.006213	0.004849	0.000001
19	H	0.004638	0.000696	0.000975	-0.002806	-0.000507	0.000000
20	H	0.001749	-0.004732	-0.000744	0.001120	0.000012	0.000000
21	H	-0.011626	0.001747	0.020403	0.016756	-0.016462	-0.004425
22	H	0.001749	-0.004732	-0.006211	0.009067	0.008844	-0.000158
23	H	0.004638	0.000696	-0.074608	0.026335	-0.017023	0.000016
24	C	-0.131483	-0.996349	-0.885543	-1.094105	-0.118081	0.000269
25	N	-0.002652	0.215708	0.022637	0.064016	0.004335	0.000001

		13	14	15	16	17	18
1	C	0.016036	0.003230	-0.041021	-0.000004	0.294864	0.014153
2	C	-0.031183	0.061249	-0.128289	0.005538	-0.016462	0.270320
3	C	0.004460	0.016772	-0.127752	-0.050920	0.016756	-0.050388
4	C	-0.015169	0.282554	-0.348825	0.008077	0.020403	0.057945
5	C	-0.041021	0.062080	-0.141943	0.002725	-0.008304	-0.031971
6	C	0.003230	-0.062553	0.062080	0.001744	0.000929	0.007803
7	C	0.014864	-0.472297	0.755107	0.339799	-0.011626	0.004478
8	C	0.017995	0.425832	-1.246587	-0.001407	0.001747	0.006583
9	C	0.175010	0.867294	-3.039736	0.008077	0.000607	0.000376

This journal is © The Royal Society of Chemistry 2014

10	C	-0.475082	-0.335544	0.841146	-0.050920	-0.001721	-0.006213
11	C	0.322714	-1.118370	1.420326	0.005539	0.000054	0.004849
12	H	0.014153	0.007803	-0.031971	0.004147	0.000000	0.000001
13	C	5.876661	0.933829	-0.727729	-0.000004	-0.000001	0.000784
14	C	0.933829	8.296960	-2.832653	0.001744	-0.000005	-0.000030
15	C	-0.727729	-2.832653	11.433278	0.002725	0.000002	0.000034
16	H	-0.000004	0.001744	0.002725	0.526664	-0.000012	0.004147
17	H	-0.000001	-0.000005	0.000002	-0.000012	0.524239	-0.004425
18	H	0.000784	-0.000030	0.000034	0.004147	-0.004425	0.534371
19	H	0.000026	0.000981	0.005570	0.000001	-0.000151	0.000016
20	H	0.000001	-0.000003	-0.000131	0.000000	-0.003900	-0.000158
21	H	0.294864	0.000929	-0.008304	-0.000012	0.000000	0.000000
22	H	-0.016741	0.304377	0.005474	0.000000	0.000000	0.000000
23	H	0.013738	0.027589	0.294304	0.000001	0.000000	0.000000
24	C	-0.001811	0.044460	0.380118	0.001236	0.000211	0.000269
25	N	-0.000499	0.030450	-0.002311	0.000008	0.000001	0.000001

		19	20	21	22	23	24
1	C	0.013738	-0.016741	-0.000001	0.000001	0.000026	-0.001811
2	C	-0.017023	0.008844	0.000054	0.000012	-0.000507	-0.118080
3	C	0.026335	0.009067	-0.001721	0.001120	-0.002806	-1.094106
4	C	-0.074608	-0.006211	0.000607	-0.000744	0.000975	-0.885542
5	C	0.294304	0.005474	0.000002	-0.000131	0.005571	0.380119
6	C	0.027589	0.304377	-0.000005	-0.000003	0.000981	0.044458
7	C	0.004638	0.001749	-0.011626	0.001749	0.004638	-0.131483
8	C	0.000696	-0.004732	0.001747	-0.004732	0.000696	-0.996349
9	C	0.000975	-0.000744	0.020403	-0.006211	-0.074608	-0.885543

This journal is © The Royal Society of Chemistry 2014

```
    10  C   -0.002806   0.001120   0.016756   0.009067   0.026335  -
1.094105
    11  C   -0.000507   0.000012  -0.016462   0.008844  -0.017023  -
0.118081
    12  H    0.000000   0.000000  -0.004425  -0.000158   0.000016
0.000269
    13  C    0.000026   0.000001   0.294864  -0.016741   0.013738  -
0.001811
    14  C    0.000981  -0.000003   0.000929   0.304377   0.027589
0.044460
    15  C    0.005570  -0.000131  -0.008304   0.005474   0.294304
0.380118
    16  H    0.000001   0.000000  -0.000012   0.000000   0.000001
0.001236
    17  H   -0.000151  -0.003900   0.000000   0.000000   0.000000
0.000211
    18  H    0.000016  -0.000158   0.000000   0.000000   0.000000
0.000269
    19  H    0.500076  -0.004176   0.000000   0.000000  -0.000001
0.005200
    20  H   -0.004176   0.521215   0.000000   0.000000   0.000000  -
0.004049
    21  H    0.000000   0.000000   0.524239  -0.003900  -0.000151
0.000211
    22  H    0.000000   0.000000  -0.003900   0.521215  -0.004176  -
0.004049
    23  H   -0.000001   0.000000  -0.000151  -0.004176   0.500076
0.005200
    24  C    0.005200  -0.004049   0.000211  -0.004049   0.005200
11.304844
    25  N    0.004975   0.000071   0.000001   0.000071   0.004975  -
0.295300
             25
     1  C   -0.000499
     2  C    0.004335
     3  C    0.064016
     4  C    0.022636
     5  C   -0.002311
     6  C    0.030450
     7  C   -0.002652
     8  C    0.215708
     9  C    0.022637
    10  C    0.064016
    11  C    0.004335
    12  H    0.000001
    13  C   -0.000499
    14  C    0.030450
    15  C   -0.002311
    16  H    0.000008
    17  H    0.000001
    18  H    0.000001
    19  H    0.004975
```

This journal is © The Royal Society of Chemistry 2014

```
   20  H    0.000071
   21  H    0.000001
   22  H    0.000071
   23  H    0.004975
   24  C   -0.295300
   25  N    7.367449
Mulliken atomic charges:
             1
    1  C   -0.379127
    2  C   -0.040118
    3  C    0.409983
    4  C    0.629111
    5  C   -0.522915
    6  C   -0.546679
    7  C   -0.009156
    8  C    0.232561
    9  C    0.629111
   10  C    0.409983
   11  C   -0.040118
   12  H    0.187055
   13  C   -0.379127
   14  C   -0.546679
   15  C   -0.522915
   16  H    0.191107
   17  H    0.186792
   18  H    0.187055
   19  H    0.214150
   20  H    0.188916
   21  H    0.186792
   22  H    0.188916
   23  H    0.214150
   24  C   -0.536286
   25  N   -0.532564
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
    1  C   -0.192334
    2  C    0.146937
    3  C    0.409983
    4  C    0.629111
    5  C   -0.308765
    6  C   -0.357763
    7  C    0.181951
    8  C    0.232561
    9  C    0.629111
   10  C    0.409983
   11  C    0.146937
   12  H    0.000000
   13  C   -0.192335
   14  C   -0.357763
   15  C   -0.308765
   16  H    0.000000
```

```
    17  H    0.000000
    18  H    0.000000
    19  H    0.000000
    20  H    0.000000
    21  H    0.000000
    22  H    0.000000
    23  H    0.000000
    24  C   -0.536286
    25  N   -0.532564
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=  3402.4169
 Charge=     0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=    -4.8121    Z=     0.0000  Tot=     4.8121
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=   -74.2319   YY=  -100.7685   ZZ=   -98.2502
   XY=     0.0000   XZ=     0.0000   YZ=     0.0000
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=    16.8516   YY=    -9.6850   ZZ=    -7.1667
   XY=     0.0000   XZ=     0.0000   YZ=     0.0000
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=     0.0000  YYY=  -101.5249  ZZZ=     0.0000  XYY=     0.0000
  XXY=    -2.6408  XXZ=     0.0000  XZZ=     0.0000  YZZ=     3.1061
  YYZ=     0.0000  XYZ=     0.0000
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX= -2770.6609 YYYY= -1774.5706 ZZZZ=  -118.2996 XXXY=     0.0000
 XXXZ=     0.0000 YYYX=     0.0001 YYYZ=     0.0000 ZZZX=     0.0000
 ZZZY=     0.0000 XXYY=  -714.7337 XXZZ=  -620.7340 YYZZ=  -289.6365
 XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
 N-N= 9.311502507686D+02 E-N=-3.324238010994D+03  KE=
6.256550219035D+02
 1\1\GINC-OPT0609\FOpt\RB3LYP\6-31+G(d)\C15H9N1\UCN0868\18-Oct-
2011\0\\
 # opt b3lyp/6-31+g(d) geom=connectivity\\cyanoanthracene\\0,1\C,-
5.600
 5017632,-0.9619117843,0.0576408591\C,-4.2293589676,-
0.9432879402,0.061
 6170612\C,-3.5114199576,0.294440262,0.0558484042\C,-
4.2534961685,1.531
 4000186,0.0457237837\C,-5.6808062969,1.4708792927,0.0418476701\C,-
6.33
 1464613,0.2615439449,0.0476357643\C,-
2.1110935035,0.3321961459,0.05978
 95673\C,-3.535498104,2.7542684938,0.040050193\C,-
2.11780676,2.78737129
 57,0.0440729375\C,-
1.3974691333,1.5376273438,0.0542144357\C,0.03317996

65,1.5634559227,0.0583224356\H,0.5685687748,0.6168425098,0.0659735506\

C,0.7158994916,2.7526818426,0.0527583832\C,0.001961872,3.9861498942,0.
```

This journal is © The Royal Society of Chemistry 2014

0427401272\C,-1.3711719193,4.0053193788,0.0385162506\H,-
1.5593413489,-
0.6060089353,0.0674357289\H,-6.1356495492,-
1.9076677684,0.0620888261\H
,-3.6623051002,-1.8712795433,0.0692435545\H,-
6.247027425,2.3976724264,
0.0342313006\H,-
7.4179176808,0.234976851,0.0445606322\H,1.8025379718,2
.7606773166,0.0559528599\H,0.5532499508,4.9227171063,0.0383989192\H,-
1
.9059181006,4.9506225134,0.0308754792\C,-
4.2609188911,3.9877816041,0.0
299973209\N,-4.8517318764,4.9924075067,0.0218098449\\Version=AM64L-
G03
RevD.01\State=1-A\HF=-631.7954329\RMSD=6.433e-09\RMSF=7.384e-
05\Therma
l=0.\Dipole=0.9597126,-1.631906,0.0132996\PG=C01 [X(C15H9N1)]\\@

... THE UNIVERSE IS NOT ONLY QUEERER THAN WE SUPPOSE,
BUT QUEERER THAN WE CAN SUPPOSE ...

-- J. B. S. HALDANE

Job cpu time: 0 days 2 hours 30 minutes 19.3 seconds.
File lengths (MBytes): RWF= 78 Int= 0 D2E= 0 Chk=
13 Scr= 1
Normal termination of Gaussian 03 at Tue Oct 18 12:52:29 2011.

This journal is © The Royal Society of Chemistry 2014

Transition state of Maleic anhydride and 9-cyanoanthracene

```
Entering Gaussian System, Link 0=g03
 Initial command:
 /usr/local/g03d01/g03/l1.exe /tmp/pbstmp.6453440/Gau-23001.inp -
scrdir=/tmp/pbstmp.6453440/
 Entering Link 1 = /usr/local/g03d01/g03/l1.exe PID=     23002.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2004, Gaussian, Inc.
                  All Rights Reserved.

 This is the Gaussian(R) 03 program.  It is based on the
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,
 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be
 used, copied, transmitted, or stored only in accord with that
 written license.

 The following legend is applicable only to US Government
 contracts under FAR:

                      RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is
 subject to restrictions as set forth in subparagraphs (a)
 and (c) of the Commercial Computer Software - Restricted
 Rights clause in FAR 52.227-19.

 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ----------------------------------------------------------------
 Warning -- This program may not be used in any manner that
 competes with the business of Gaussian, Inc. or will provide
 assistance to any competitor of Gaussian, Inc.  The licensee
 of this program is prohibited from giving any competitor of
 Gaussian, Inc. access to this program.  By using this program,
 the user acknowledges that Gaussian, Inc. is engaged in the
```

```
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.
----------------------------------------------------------------


Cite this work as:
Gaussian 03, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.

****************************************
Gaussian 03:  AM64L-G03RevD.01 13-Oct-2005
               27-Sep-2011
****************************************
%chk=daant.chk
%mem=6MW
%nprocshared=1
Will use up to    1 processors via shared memory.
----------------------------------------------------
# opt=(calcfc,ts) b3lyp/6-31+g(d) geom=connectivity
----------------------------------------------------
1/5=1,10=4,14=-1,18=20,26=3,38=1,57=2/1,3;
2/9=110,17=6,18=5,40=1/2;
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,7=6/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/10=1,18=20,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20/3(3);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
```

This journal is © The Royal Society of Chemistry 2014

```
99//99;
2/9=110/2;
3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,74=-5/1,2,3;
4/5=5,16=3/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/5=1,14=-1,18=20/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
--------------
cyanoDFT6-31+d
--------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                    -0.55176   1.12346  -0.71154
C                     0.52135   0.41324  -1.35441
C                    -0.55178   1.12349   0.71147
C                     0.52132   0.4133    1.3544
H                     0.48802   0.32044   2.4385
C                    -0.01512  -1.63551   0.70583
H                     0.74921  -2.0749    1.33282
C                    -0.0151   -1.63554  -0.70576
H                     0.74924  -2.07496  -1.33271
C                    -1.62973   1.71557  -1.40845
H                    -1.64087   1.69181  -2.49503
C                    -2.65443   2.32608  -0.70629
H                    -3.47226   2.79793  -1.24395
C                    -2.65445   2.32611   0.70612
H                    -3.47229   2.79799   1.24372
C                    -1.62977   1.71564   1.40833
H                    -1.64094   1.69193   2.49491
C                     1.81088   0.38002   0.71069
C                     1.8109    0.37998  -0.71066
C                     3.03221   0.24162  -1.40633
H                     3.03001   0.23046  -2.49398
C                     4.22403   0.14268  -0.70593
H                     5.1645    0.0622   -1.24443
C                     4.22402   0.14271   0.70604
H                     5.16446   0.06226   1.24457
C                     3.03218   0.24169   1.40641
H                     3.02994   0.23057   2.49405
C                    -1.42897  -1.71085  -1.13993
C                    -1.429    -1.7108    1.13997
O                    -2.23652  -1.63957   0.00001
O                    -1.90288  -1.806     2.2424
O                    -1.90282  -1.8061   -2.24237
C                     0.4743    0.28179  -2.88807
N                     0.43926   0.18392  -4.02994
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Initialization pass.
                           ----------------------------
                           !    Initial Parameters    !
                           ! (Angstroms and Degrees)  !
 --------------------------                            ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ---------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.4385         calculate D2E/DX2
analytically  !
 ! R2    R(1,3)                  1.423          calculate D2E/DX2
analytically  !
 ! R3    R(1,8)                  2.8107         calculate D2E/DX2
analytically  !
 ! R4    R(1,10)                 1.4136         calculate D2E/DX2
analytically  !
 ! R5    R(2,8)                  2.215          calculate D2E/DX2
analytically  !
 ! R6    R(2,9)                  2.4987         calculate D2E/DX2
analytically  !
 ! R7    R(2,19)                 1.4417         calculate D2E/DX2
analytically  !
 ! R8    R(2,33)                 1.54           calculate D2E/DX2
analytically  !
 ! R9    R(3,4)                  1.4385         calculate D2E/DX2
analytically  !
 ! R10   R(3,6)                  2.8107         calculate D2E/DX2
analytically  !
 ! R11   R(3,16)                 1.4136         calculate D2E/DX2
analytically  !
 ! R12   R(4,5)                  1.0886         calculate D2E/DX2
analytically  !
 ! R13   R(4,6)                  2.215          calculate D2E/DX2
analytically  !
 ! R14   R(4,7)                  2.4987         calculate D2E/DX2
analytically  !
 ! R15   R(4,18)                 1.4417         calculate D2E/DX2
analytically  !
 ! R16   R(5,6)                  2.661          calculate D2E/DX2
analytically  !
 ! R17   R(6,7)                  1.0818         calculate D2E/DX2
analytically  !
 ! R18   R(6,8)                  1.4116         calculate D2E/DX2
analytically  !
 ! R19   R(6,18)                 2.7197         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R20   R(6,29)                 1.4809         calculate D2E/DX2
analytically  !
 ! R21   R(7,18)                 2.746          calculate D2E/DX2
analytically  !
 ! R22   R(8,9)                  1.0818         calculate D2E/DX2
analytically  !
 ! R23   R(8,19)                 2.7197         calculate D2E/DX2
analytically  !
 ! R24   R(8,28)                 1.4809         calculate D2E/DX2
analytically  !
 ! R25   R(9,19)                 2.746          calculate D2E/DX2
analytically  !
 ! R26   R(9,33)                 2.8371         calculate D2E/DX2
analytically  !
 ! R27   R(10,11)                1.0869         calculate D2E/DX2
analytically  !
 ! R28   R(10,12)                1.3841         calculate D2E/DX2
analytically  !
 ! R29   R(12,13)                1.0865         calculate D2E/DX2
analytically  !
 ! R30   R(12,14)                1.4124         calculate D2E/DX2
analytically  !
 ! R31   R(14,15)                1.0865         calculate D2E/DX2
analytically  !
 ! R32   R(14,16)                1.3841         calculate D2E/DX2
analytically  !
 ! R33   R(16,17)                1.0869         calculate D2E/DX2
analytically  !
 ! R34   R(18,19)                1.4213         calculate D2E/DX2
analytically  !
 ! R35   R(18,26)                1.4123         calculate D2E/DX2
analytically  !
 ! R36   R(19,20)                1.4123         calculate D2E/DX2
analytically  !
 ! R37   R(20,21)                1.0877         calculate D2E/DX2
analytically  !
 ! R38   R(20,22)                1.3859         calculate D2E/DX2
analytically  !
 ! R39   R(22,23)                1.0867         calculate D2E/DX2
analytically  !
 ! R40   R(22,24)                1.412          calculate D2E/DX2
analytically  !
 ! R41   R(24,25)                1.0867         calculate D2E/DX2
analytically  !
 ! R42   R(24,26)                1.3859         calculate D2E/DX2
analytically  !
 ! R43   R(26,27)                1.0877         calculate D2E/DX2
analytically  !
 ! R44   R(28,30)                1.3988         calculate D2E/DX2
analytically  !
 ! R45   R(28,32)                1.2037         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R46   R(29,30)              1.3988         calculate D2E/DX2
analytically  !
 ! R47   R(29,31)              1.2037         calculate D2E/DX2
analytically  !
 ! R48   R(33,34)              1.1466         calculate D2E/DX2
analytically  !
 ! A1    A(2,1,3)             116.5467         calculate D2E/DX2
analytically  !
 ! A2    A(2,1,10)            123.7349         calculate D2E/DX2
analytically  !
 ! A3    A(3,1,10)            119.5365         calculate D2E/DX2
analytically  !
 ! A4    A(1,2,19)            118.6273         calculate D2E/DX2
analytically  !
 ! A5    A(1,2,33)            117.6722         calculate D2E/DX2
analytically  !
 ! A6    A(19,2,33)           118.0374         calculate D2E/DX2
analytically  !
 ! A7    A(1,3,4)             116.5467         calculate D2E/DX2
analytically  !
 ! A8    A(1,3,16)            119.5366         calculate D2E/DX2
analytically  !
 ! A9    A(4,3,16)            123.7349         calculate D2E/DX2
analytically  !
 ! A10   A(3,4,5)             117.6722         calculate D2E/DX2
analytically  !
 ! A11   A(3,4,18)            118.6273         calculate D2E/DX2
analytically  !
 ! A12   A(5,4,18)            118.0376         calculate D2E/DX2
analytically  !
 ! A13   A(7,6,8)             125.4181         calculate D2E/DX2
analytically  !
 ! A14   A(7,6,29)            118.9449         calculate D2E/DX2
analytically  !
 ! A15   A(8,6,29)            107.0473         calculate D2E/DX2
analytically  !
 ! A16   A(6,8,9)             125.4181         calculate D2E/DX2
analytically  !
 ! A17   A(6,8,28)            107.0473         calculate D2E/DX2
analytically  !
 ! A18   A(9,8,28)            118.9449         calculate D2E/DX2
analytically  !
 ! A19   A(1,10,11)           119.4399         calculate D2E/DX2
analytically  !
 ! A20   A(1,10,12)           119.9476         calculate D2E/DX2
analytically  !
 ! A21   A(11,10,12)          120.6112         calculate D2E/DX2
analytically  !
 ! A22   A(10,12,13)          119.8523         calculate D2E/DX2
analytically  !
 ! A23   A(10,12,14)          120.4855         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A24   A(13,12,14)           119.6573         calculate D2E/DX2
analytically  !
 ! A25   A(12,14,15)           119.6574         calculate D2E/DX2
analytically  !
 ! A26   A(12,14,16)           120.4855         calculate D2E/DX2
analytically  !
 ! A27   A(15,14,16)           119.8522         calculate D2E/DX2
analytically  !
 ! A28   A(3,16,14)            119.9475         calculate D2E/DX2
analytically  !
 ! A29   A(3,16,17)            119.4399         calculate D2E/DX2
analytically  !
 ! A30   A(14,16,17)           120.6112         calculate D2E/DX2
analytically  !
 ! A31   A(4,18,19)            116.5202         calculate D2E/DX2
analytically  !
 ! A32   A(4,18,26)            123.7661         calculate D2E/DX2
analytically  !
 ! A33   A(19,18,26)           119.5105         calculate D2E/DX2
analytically  !
 ! A34   A(2,19,18)            116.5202         calculate D2E/DX2
analytically  !
 ! A35   A(2,19,20)            123.7661         calculate D2E/DX2
analytically  !
 ! A36   A(18,19,20)           119.5105         calculate D2E/DX2
analytically  !
 ! A37   A(19,20,21)           119.4585         calculate D2E/DX2
analytically  !
 ! A38   A(19,20,22)           120.1121         calculate D2E/DX2
analytically  !
 ! A39   A(21,20,22)           120.4214         calculate D2E/DX2
analytically  !
 ! A40   A(20,22,23)           119.9388         calculate D2E/DX2
analytically  !
 ! A41   A(20,22,24)           120.3551         calculate D2E/DX2
analytically  !
 ! A42   A(23,22,24)           119.706          calculate D2E/DX2
analytically  !
 ! A43   A(22,24,25)           119.706          calculate D2E/DX2
analytically  !
 ! A44   A(22,24,26)           120.355          calculate D2E/DX2
analytically  !
 ! A45   A(25,24,26)           119.9388         calculate D2E/DX2
analytically  !
 ! A46   A(18,26,24)           120.1122         calculate D2E/DX2
analytically  !
 ! A47   A(18,26,27)           119.4585         calculate D2E/DX2
analytically  !
 ! A48   A(24,26,27)           120.4213         calculate D2E/DX2
analytically  !
 ! A49   A(8,28,30)            108.0383         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A50   A(8,28,32)            130.4169         calculate D2E/DX2
analytically  !
 ! A51   A(30,28,32)           121.5426         calculate D2E/DX2
analytically  !
 ! A52   A(6,29,30)            108.0383         calculate D2E/DX2
analytically  !
 ! A53   A(6,29,31)            130.417          calculate D2E/DX2
analytically  !
 ! A54   A(30,29,31)           121.5426         calculate D2E/DX2
analytically  !
 ! A55   A(28,30,29)           109.1635         calculate D2E/DX2
analytically  !
 ! A56   L(2,33,34,1,-1)       180.0            calculate D2E/DX2
analytically  !
 ! A57   L(2,33,34,1,-2)       180.0            calculate D2E/DX2
analytically  !
 ! D1    D(3,1,2,19)           -32.717          calculate D2E/DX2
analytically  !
 ! D2    D(3,1,2,33)           174.2954         calculate D2E/DX2
analytically  !
 ! D3    D(10,1,2,19)          152.2192         calculate D2E/DX2
analytically  !
 ! D4    D(10,1,2,33)           -0.7684         calculate D2E/DX2
analytically  !
 ! D5    D(2,1,3,4)              0.0            calculate D2E/DX2
analytically  !
 ! D6    D(2,1,3,16)          -175.2824         calculate D2E/DX2
analytically  !
 ! D7    D(10,1,3,4)           175.2824         calculate D2E/DX2
analytically  !
 ! D8    D(10,1,3,16)            0.0            calculate D2E/DX2
analytically  !
 ! D9    D(2,1,10,11)           -3.4913         calculate D2E/DX2
analytically  !
 ! D10   D(2,1,10,12)          176.9192         calculate D2E/DX2
analytically  !
 ! D11   D(3,1,10,11)         -178.4155         calculate D2E/DX2
analytically  !
 ! D12   D(3,1,10,12)            1.995          calculate D2E/DX2
analytically  !
 ! D13   D(1,2,19,18)           32.7085         calculate D2E/DX2
analytically  !
 ! D14   D(1,2,19,20)         -152.5105         calculate D2E/DX2
analytically  !
 ! D15   D(33,2,19,18)        -174.4025         calculate D2E/DX2
analytically  !
 ! D16   D(33,2,19,20)           0.3785         calculate D2E/DX2
analytically  !
 ! D17   D(1,3,4,5)           -174.2953         calculate D2E/DX2
analytically  !
 ! D18   D(1,3,4,18)            32.7169         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D19   D(16,3,4,5)             0.7686         calculate D2E/DX2
analytically  !
 ! D20   D(16,3,4,18)         -152.2192         calculate D2E/DX2
analytically  !
 ! D21   D(1,3,16,14)           -1.9949         calculate D2E/DX2
analytically  !
 ! D22   D(1,3,16,17)          178.4155         calculate D2E/DX2
analytically  !
 ! D23   D(4,3,16,14)         -176.9193         calculate D2E/DX2
analytically  !
 ! D24   D(4,3,16,17)            3.4912         calculate D2E/DX2
analytically  !
 ! D25   D(3,4,18,19)          -32.7084         calculate D2E/DX2
analytically  !
 ! D26   D(3,4,18,26)          152.5105         calculate D2E/DX2
analytically  !
 ! D27   D(5,4,18,19)          174.4024         calculate D2E/DX2
analytically  !
 ! D28   D(5,4,18,26)           -0.3787         calculate D2E/DX2
analytically  !
 ! D29   D(7,6,8,9)              0.0001         calculate D2E/DX2
analytically  !
 ! D30   D(7,6,8,28)           147.0577         calculate D2E/DX2
analytically  !
 ! D31   D(29,6,8,9)          -147.0575         calculate D2E/DX2
analytically  !
 ! D32   D(29,6,8,28)            0.0            calculate D2E/DX2
analytically  !
 ! D33   D(7,6,29,30)         -154.4955         calculate D2E/DX2
analytically  !
 ! D34   D(7,6,29,31)           26.0525         calculate D2E/DX2
analytically  !
 ! D35   D(8,6,29,30)           -4.9213         calculate D2E/DX2
analytically  !
 ! D36   D(8,6,29,31)          175.6267         calculate D2E/DX2
analytically  !
 ! D37   D(6,8,28,30)            4.9213         calculate D2E/DX2
analytically  !
 ! D38   D(6,8,28,32)         -175.6267         calculate D2E/DX2
analytically  !
 ! D39   D(9,8,28,30)          154.4954         calculate D2E/DX2
analytically  !
 ! D40   D(9,8,28,32)          -26.0526         calculate D2E/DX2
analytically  !
 ! D41   D(1,10,12,13)         178.7897         calculate D2E/DX2
analytically  !
 ! D42   D(1,10,12,14)          -2.0141         calculate D2E/DX2
analytically  !
 ! D43   D(11,10,12,13)         -0.7949         calculate D2E/DX2
analytically  !
 ! D44   D(11,10,12,14)        178.4012         calculate D2E/DX2
analytically  !
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D45   D(10,12,14,15)       -179.1977         calculate D2E/DX2
analytically  !
 ! D46   D(10,12,14,16)          0.0            calculate D2E/DX2
analytically  !
 ! D47   D(13,12,14,15)          0.0            calculate D2E/DX2
analytically  !
 ! D48   D(13,12,14,16)        179.1978         calculate D2E/DX2
analytically  !
 ! D49   D(12,14,16,3)           2.0141         calculate D2E/DX2
analytically  !
 ! D50   D(12,14,16,17)       -178.4012         calculate D2E/DX2
analytically  !
 ! D51   D(15,14,16,3)        -178.7897         calculate D2E/DX2
analytically  !
 ! D52   D(15,14,16,17)          0.795          calculate D2E/DX2
analytically  !
 ! D53   D(4,18,19,2)           -0.0001         calculate D2E/DX2
analytically  !
 ! D54   D(4,18,19,20)        -175.0153         calculate D2E/DX2
analytically  !
 ! D55   D(26,18,19,2)         175.0152         calculate D2E/DX2
analytically  !
 ! D56   D(26,18,19,20)          0.0            calculate D2E/DX2
analytically  !
 ! D57   D(4,18,26,24)         176.3459         calculate D2E/DX2
analytically  !
 ! D58   D(4,18,26,27)          -4.6815         calculate D2E/DX2
analytically  !
 ! D59   D(19,18,26,24)          1.7121         calculate D2E/DX2
analytically  !
 ! D60   D(19,18,26,27)       -179.3152         calculate D2E/DX2
analytically  !
 ! D61   D(2,19,20,21)           4.6816         calculate D2E/DX2
analytically  !
 ! D62   D(2,19,20,22)        -176.3458         calculate D2E/DX2
analytically  !
 ! D63   D(18,19,20,21)        179.3152         calculate D2E/DX2
analytically  !
 ! D64   D(18,19,20,22)         -1.7122         calculate D2E/DX2
analytically  !
 ! D65   D(19,20,22,23)       -178.4179         calculate D2E/DX2
analytically  !
 ! D66   D(19,20,22,24)          1.7268         calculate D2E/DX2
analytically  !
 ! D67   D(21,20,22,23)          0.5447         calculate D2E/DX2
analytically  !
 ! D68   D(21,20,22,24)       -179.3106         calculate D2E/DX2
analytically  !
 ! D69   D(20,22,24,25)        179.8557         calculate D2E/DX2
analytically  !
 ! D70   D(20,22,24,26)          0.0            calculate D2E/DX2
analytically  !
```

```
 ! D71   D(23,22,24,25)          0.0001         calculate D2E/DX2
analytically  !
 ! D72   D(23,22,24,26)       -179.8556         calculate D2E/DX2
analytically  !
 ! D73   D(22,24,26,18)         -1.7268         calculate D2E/DX2
analytically  !
 ! D74   D(22,24,26,27)        179.3106         calculate D2E/DX2
analytically  !
 ! D75   D(25,24,26,18)        178.4179         calculate D2E/DX2
analytically  !
 ! D76   D(25,24,26,27)         -0.5448         calculate D2E/DX2
analytically  !
 ! D77   D(8,28,30,29)          -8.1359         calculate D2E/DX2
analytically  !
 ! D78   D(32,28,30,29)        172.3535         calculate D2E/DX2
analytically  !
 ! D79   D(6,29,30,28)           8.136          calculate D2E/DX2
analytically  !
 ! D80   D(31,29,30,28)       -172.3536         calculate D2E/DX2
analytically  !
 ---------------------------------------------------------------------
-----------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
 Number of steps in this run= 195 maximum allowed number of steps=
204.
 Search for a saddle point of order  1.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.551761    1.123457   -0.711538
    2          6             0        0.521350    0.413239   -1.354407
    3          6             0       -0.551780    1.123491    0.711472
    4          6             0        0.521315    0.413304    1.354404
    5          1             0        0.488023    0.320438    2.438497
    6          6             0       -0.015123   -1.635507    0.705829
    7          1             0        0.749209   -2.074896    1.332819
    8          6             0       -0.015104   -1.635538   -0.705756
    9          1             0        0.749244   -2.074956   -1.332705
   10          6             0       -1.629734    1.715571   -1.408448
   11          1             0       -1.640870    1.691809   -2.495026
   12          6             0       -2.654427    2.326075   -0.706294
   13          1             0       -3.472257    2.797925   -1.243947
   14          6             0       -2.654446    2.326109    0.706115
   15          1             0       -3.472290    2.797985    1.243724
   16          6             0       -1.629771    1.715639    1.408326
   17          1             0       -1.640936    1.691929    2.494905
```

18	6	0	1.810882	0.380015	0.710689
19	6	0	1.810901	0.379982	-0.710656
20	6	0	3.032215	0.241620	-1.406334
21	1	0	3.030007	0.230455	-2.493977
22	6	0	4.224035	0.142680	-0.705928
23	1	0	5.164497	0.062196	-1.244431
24	6	0	4.224016	0.142713	0.706036
25	1	0	5.164464	0.062255	1.244567
26	6	0	3.032177	0.241686	1.406405
27	1	0	3.029941	0.230571	2.494048
28	6	0	-1.428972	-1.710850	-1.139929
29	6	0	-1.429002	-1.710801	1.139968
30	8	0	-2.236516	-1.639571	0.000007
31	8	0	-1.902882	-1.805999	2.242403
32	8	0	-1.902822	-1.806096	-2.242372
33	6	0	0.474296	0.281791	-2.888065
34	7	0	0.439262	0.183922	-4.029943

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.438491	0.000000			
3	C	1.423010	2.433911	0.000000		
4	C	2.433912	2.708811	1.438492	0.000000	
5	H	3.413021	3.794185	2.169954	1.088572	0.000000
6	C	3.147823	2.954613	2.810712	2.214959	2.661018
7	H	4.012653	3.669321	3.508322	2.498708	2.651107
8	C	2.810709	2.214953	3.147824	2.954616	3.737018
9	H	3.508320	2.498704	4.012653	3.669325	4.475278
10	C	1.413615	2.515184	2.450837	3.735808	4.607632
11	H	2.165644	2.758795	3.433764	4.596491	5.545493
12	C	2.422297	3.763582	2.806669	4.241522	4.877221
13	H	3.408313	4.652722	3.893145	5.327895	5.948290
14	C	2.806670	4.241521	2.422297	3.763583	4.110836
15	H	3.893146	5.327894	3.408314	4.652723	4.821805
16	C	2.450838	3.735808	1.413616	2.515185	2.737314
17	H	3.433765	4.596491	2.165644	2.758796	2.533108
18	C	2.856137	2.434875	2.476879	1.441687	2.176884
19	C	2.476879	1.441688	2.856136	2.434875	3.416243
20	C	3.755697	2.517259	4.255328	3.735742	4.611057
21	H	4.099220	2.761411	4.888928	4.597500	5.549692
22	C	4.875467	3.768767	5.077344	4.245979	4.886388
23	H	5.838309	4.657697	6.134144	5.332575	5.958192
24	C	5.077344	4.245980	4.875467	3.768766	4.121972
25	H	6.134144	5.332576	5.838309	4.657696	4.833345
26	C	4.255328	3.735742	3.755697	2.517257	2.746659
27	H	4.888928	4.597500	4.099220	2.761410	2.544113
28	C	2.997718	2.891628	3.497233	3.812787	4.539398
29	C	3.497234	3.812784	2.997722	2.891633	3.080113
30	O	3.313460	3.695171	3.313462	3.695175	4.148612
31	O	4.374129	4.872264	3.570874	3.404494	3.205716
32	O	3.570868	3.404488	4.374127	4.872266	5.669993

This journal is © The Royal Society of Chemistry 2014

33	C	2.549209	1.540000	3.836399	4.244767	5.326720
34	N	3.588407	2.686600	4.934164	5.389856	6.470065
		6	7	8	9	10
6	C	0.000000				
7	H	1.081842	0.000000			
8	C	1.411585	2.221035	0.000000		
9	H	2.221034	2.665524	1.081842	0.000000	
10	C	4.278652	5.248005	3.785596	4.475865	0.000000
11	H	4.894850	5.878175	4.112887	4.610006	1.086895
12	C	4.965294	5.925476	4.760295	5.598789	1.384099
13	H	5.950523	6.942974	5.647756	6.447784	2.143232
14	C	4.760297	5.598792	4.965295	5.925476	2.427791
15	H	5.647759	6.447787	5.950524	6.942974	3.405973
16	C	3.785600	4.475869	4.278654	5.248007	2.816774
17	H	4.112893	4.610012	4.894854	5.878178	3.903441
18	C	2.719678	2.746049	3.066430	3.365920	4.255854
19	C	3.066429	3.365918	2.719676	2.746048	3.756152
20	C	4.155852	4.252214	3.647010	3.253291	4.889407
21	H	4.795142	5.016079	3.994041	3.444612	5.009703
22	C	4.808895	4.598755	4.596995	4.169524	6.101978
23	H	5.789143	5.541132	5.477293	4.906085	6.994435
24	C	4.596995	4.169524	4.808895	4.598756	6.419604
25	H	5.477295	4.906086	5.789144	5.541134	7.478841
26	C	3.647012	3.253292	4.155853	4.252216	5.641733
27	H	3.994044	3.444615	4.795144	5.016081	6.256778
28	C	2.326256	3.315341	1.480946	2.216836	3.442785
29	C	1.480946	2.216836	2.326256	3.315340	4.274897
30	O	2.330834	3.298553	2.330834	3.298552	3.689025
31	O	2.440033	2.816600	3.504911	4.459541	5.079840
32	O	3.504910	4.459542	2.440032	2.816600	3.629345
33	C	4.102638	4.842047	2.945868	2.837076	2.944815
34	N	5.093557	5.827310	3.816688	3.531815	3.674089
		11	12	13	14	15
11	H	0.000000				
12	C	2.151547	0.000000			
13	H	2.478441	1.086535	0.000000		
14	C	3.417159	1.412409	2.166603	0.000000	
15	H	4.307665	2.166603	2.487671	1.086535	0.000000
16	C	3.903441	2.427791	3.405973	1.384100	2.143232
17	H	4.989931	3.417160	4.307665	2.151547	2.478441
18	C	4.889990	5.072867	6.130126	4.870981	5.834605
19	C	4.101169	4.870981	5.834604	5.072866	6.130126
20	C	5.012586	6.096959	6.990652	6.414487	7.474383
21	H	4.894144	6.316662	7.101684	6.851668	7.927325
22	C	6.324380	7.216679	8.159210	7.353552	8.371691
23	H	7.108632	8.157837	9.059676	8.370532	9.395187
24	C	6.858818	7.353552	8.371691	7.216679	8.159210
25	H	7.934266	8.370531	9.395187	8.157838	9.059677
26	C	6.257906	6.414487	7.474382	6.096959	6.990652
27	H	6.988745	6.851669	7.927326	6.316664	7.101685
28	C	3.668689	4.241054	4.951251	4.605074	5.494228
29	C	4.983555	4.605075	5.494229	4.241059	4.951257

30	O	4.204530	4.049674	4.771357	4.049676	4.771360
31	O	5.894620	5.131634	5.984454	4.472063	4.965589
32	O	3.516787	4.472056	4.965580	5.131631	5.984451
33	C	2.572267	4.327601	4.960780	5.185209	6.243273
34	N	2.992765	5.020595	5.467611	6.048987	7.067187
		16	17	18	19	20
16	C	0.000000				
17	H	1.086895	0.000000			
18	C	3.756153	4.101170	0.000000		
19	C	4.255853	4.889990	1.421345	0.000000	
20	C	5.641733	6.257907	2.447978	1.412345	0.000000
21	H	6.256778	6.988745	3.431985	2.165366	1.087703
22	C	6.419604	6.858818	2.808280	2.424778	1.385927
23	H	7.478842	7.934266	3.894899	3.410647	2.145934
24	C	6.101978	6.324380	2.424778	2.808280	2.427402
25	H	6.994435	7.108632	3.410646	3.894898	3.406748
26	C	4.889407	5.012586	1.412345	2.447976	2.812739
27	H	5.009704	4.894145	2.165365	3.431983	3.900398
28	C	4.274898	4.983558	4.277050	3.879772	4.877018
29	C	3.442792	3.668698	3.879773	4.277050	5.495276
30	O	3.689029	4.204536	4.578780	4.578779	5.768553
31	O	3.629354	3.516799	4.573494	5.224103	6.470024
32	O	5.079840	5.894621	5.224103	4.573492	5.408021
33	C	4.994196	5.953072	3.840201	2.556808	2.956365
34	N	6.016795	7.012486	4.938966	3.596874	3.689182
		21	22	23	24	25
21	H	0.000000				
22	C	2.151866	0.000000			
23	H	2.479057	1.086707	0.000000		
24	C	3.416642	1.411964	2.166866	0.000000	
25	H	4.308237	2.166865	2.488998	1.086707	0.000000
26	C	3.900399	2.427402	3.406749	1.385927	2.145934
27	H	4.988025	3.416640	4.308237	2.151865	2.479057
28	C	5.048228	5.964932	6.828502	6.228929	7.232090
29	C	6.070980	6.228929	7.232089	5.964933	6.828504
30	O	6.119903	6.738953	7.695429	6.738953	7.695430
31	O	7.135393	7.073126	8.099136	6.610354	7.377901
32	O	5.342625	6.610353	7.377899	7.073126	8.099136
33	C	2.586426	4.340693	4.974710	5.195893	6.254960
34	N	3.012195	5.037389	5.486506	6.062637	7.082570
		26	27	28	29	30
26	C	0.000000				
27	H	1.087702	0.000000			
28	C	5.495277	6.070981	0.000000		
29	C	4.877019	5.048230	2.279897	0.000000	
30	O	5.768553	6.119905	1.398807	1.398808	0.000000
31	O	5.408023	5.342629	3.416696	1.203739	2.273181
32	O	6.470023	7.135393	1.203738	3.416696	2.273180
33	C	4.998684	5.958279	3.263285	4.880371	4.402396
34	N	6.023324	7.019705	3.928440	5.814496	5.169663
		31	32	33	34	
31	O	0.000000				

```
   32  O    4.484775   0.000000
   33  C    6.027565   3.229068   0.000000
   34  N    6.984823   3.555410   1.146600   0.000000
 Stoichiometry    C19H11NO3
 Framework group  C1[X(C19H11NO3)]
 Deg. of freedom    96
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.557756    0.562516    1.063099
    2          6             0        0.546248    1.080539    0.300155
    3          6             0       -0.635611   -0.852812    1.188573
    4          6             0        0.398046   -1.613649    0.539004
    5          1             0        0.305158   -2.698247    0.542027
    6          6             0       -0.109773   -1.119624   -1.559592
    7          1             0        0.617471   -1.823829   -1.941161
    8          6             0       -0.032542    0.284340   -1.684055
    9          1             0        0.763306    0.827305   -2.176189
   10          6             0       -1.593773    1.366908    1.590291
   11          1             0       -1.545547    2.446140    1.470827
   12          6             0       -2.653048    0.778483    2.259189
   13          1             0       -3.438474    1.399625    2.680910
   14          6             0       -2.730324   -0.626301    2.383728
   15          1             0       -3.574579   -1.074616    2.900260
   16          6             0       -1.747883   -1.434660    1.838660
   17          1             0       -1.818554   -2.516852    1.910813
   18          6             0        1.720759   -1.047027    0.450516
   19          6             0        1.798523    0.366645    0.325190
   20          6             0        3.055535    0.979436    0.127382
   21          1             0        3.112781    2.060348    0.020382
   22          6             0        4.206881    0.208764    0.091877
   23          1             0        5.175083    0.685721   -0.034731
   24          6             0        4.129630   -1.195577    0.216376
   25          1             0        5.038906   -1.789840    0.184736
   26          6             0        2.901645   -1.818118    0.375394
   27          1             0        2.839878   -2.900749    0.460196
   28          6             0       -1.420817    0.787039   -1.798899
   29          6             0       -1.545553   -1.480550   -1.597875
   30          8             0       -2.289232   -0.296202   -1.628297
   31          8             0       -2.079378   -2.559446   -1.596041
   32          8             0       -1.834008    1.901118   -1.991475
   33          6             0        0.582662    2.596923    0.033973
   34          7             0        0.609774    3.725940   -0.164211
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3936465      0.2684450
0.2448201
 Standard basis: 6-31+G(d) (6D, 7F)
```

This journal is © The Royal Society of Chemistry 2014

```
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1867.2825415379 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1011.05199973     A.U. after   18 cycles
             Convg  =    0.2429D-08             -V/T =  2.0094
             S**2   =   0.0000
 Range of M.O.s used for correlation:     1   454
 NBasis=   459 NAE=    78 NBE=    78 NFC=     0 NFV=     0
 NROrb=    454 NOA=    78 NOB=    78 NVA=   376 NVB=   376

 **** Warning!!: The largest alpha MO coefficient is  0.15226618D+03

 Symmetrizing basis deriv contribution to polar:
 IMax=3 JMax=2 DiffMx= 0.00D+00
 G2DrvN: will do    4 centers at a time, making    9 passes doing
MaxLOS=2.
 FoFDir/FoFCou used for L=0 through L=2.
 DoAtom=TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT
          Differentiating once with respect to electric field.
                with respect to dipole field.
          Differentiating once with respect to nuclear coordinates.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 2 Meth= 1.
 IRaf=       0 NMat=  18 IRICut=      18 DoRegI=T DoRafI=T ISym2E= 2
JSym2E=2.
          There are 105 degrees of freedom in the 1st order CPHF.
   105 vectors were produced by pass  0.
 AX will form  18 AO Fock derivatives at one time.
   102 vectors were produced by pass  1.
   102 vectors were produced by pass  2.
   102 vectors were produced by pass  3.
    96 vectors were produced by pass  4.
    52 vectors were produced by pass  5.
     5 vectors were produced by pass  6.
     2 vectors were produced by pass  7.
 Inv2:  IOpt= 1 Iter= 1 AM= 3.15D-15 Conv= 1.00D-12.
 Inverted reduced A of dimension  566 with in-core refinement.
 Isotropic polarizability for W=    0.000000      240.41 Bohr**3.
 End of Minotr Frequency-dependent properties file   721 does not
exist.


**********************************************************************
```

```
          Population analysis using the SCF density.

**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.22684 -19.17436 -19.17250 -14.36143 -
10.34747
 Alpha  occ. eigenvalues --  -10.34565 -10.29509 -10.26176 -10.25508 -
10.25091
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha  occ. eigenvalues --  -10.24871 -10.24671 -10.24354 -10.24335 -
10.24005
 Alpha  occ. eigenvalues --  -10.23233 -10.23046 -10.23003 -10.22949 -
10.22509
 Alpha  occ. eigenvalues --  -10.22316 -10.22283 -10.22236  -1.14564
-1.08134
 Alpha  occ. eigenvalues --   -1.04289  -0.94164  -0.92614  -0.88965
-0.85214
 Alpha  occ. eigenvalues --   -0.83350  -0.82768  -0.78718  -0.78011
-0.74677
 Alpha  occ. eigenvalues --   -0.70730  -0.69239  -0.65848  -0.65067
-0.63809
 Alpha  occ. eigenvalues --   -0.63110  -0.59367  -0.58371  -0.55964
-0.55634
 Alpha  occ. eigenvalues --   -0.51761  -0.51390  -0.50748  -0.50221
-0.49618
 Alpha  occ. eigenvalues --   -0.48466  -0.48004  -0.46447  -0.46150
-0.45871
 Alpha  occ. eigenvalues --   -0.45135  -0.44762  -0.44678  -0.43392
-0.42387
 Alpha  occ. eigenvalues --   -0.41165  -0.41050  -0.39491  -0.38884
-0.38356
 Alpha  occ. eigenvalues --   -0.38002  -0.37879  -0.36875  -0.35980
-0.35724
 Alpha  occ. eigenvalues --   -0.33787  -0.33033  -0.32039  -0.29565
-0.28775
 Alpha  occ. eigenvalues --   -0.28073  -0.27870  -0.25234
 Alpha virt. eigenvalues --   -0.10880  -0.09558  -0.04817  -0.04003
-0.03359
 Alpha virt. eigenvalues --   -0.01305  -0.01025  -0.00127   0.00335
0.00638
 Alpha virt. eigenvalues --    0.01041   0.01934   0.01962   0.02367
0.02975
 Alpha virt. eigenvalues --    0.03307   0.03575   0.04143   0.04465
0.05667
 Alpha virt. eigenvalues --    0.05828   0.06043   0.06312   0.06426
0.06499
 Alpha virt. eigenvalues --    0.07376   0.07885   0.08283   0.08820
0.09355
 Alpha virt. eigenvalues --    0.09974   0.10085   0.10265   0.10493
0.10770
 Alpha virt. eigenvalues --    0.11336   0.11809   0.12086   0.12272
0.13136
 Alpha virt. eigenvalues --    0.13278   0.13739   0.13868   0.14031
0.14509
 Alpha virt. eigenvalues --    0.14929   0.15496   0.15656   0.15968
0.16490
 Alpha virt. eigenvalues --    0.16602   0.16843   0.17100   0.17287
0.17633
 Alpha virt. eigenvalues --    0.17905   0.18440   0.18596   0.18986
0.19093
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.19647   0.19865   0.20137   0.20320
0.20677
 Alpha virt. eigenvalues --    0.21202   0.21833   0.22084   0.22278
0.22408
 Alpha virt. eigenvalues --    0.22585   0.22909   0.23135   0.23590
0.24126
 Alpha virt. eigenvalues --    0.24431   0.24529   0.24707   0.25638
0.25778
 Alpha virt. eigenvalues --    0.26062   0.26235   0.26408   0.26726
0.27111
 Alpha virt. eigenvalues --    0.27408   0.27481   0.28093   0.28159
0.28340
 Alpha virt. eigenvalues --    0.28645   0.28989   0.29156   0.29450
0.29710
 Alpha virt. eigenvalues --    0.29990   0.30280   0.30841   0.31200
0.32586
 Alpha virt. eigenvalues --    0.33417   0.33702   0.34210   0.34428
0.34818
 Alpha virt. eigenvalues --    0.34949   0.35556   0.35625   0.35815
0.36332
 Alpha virt. eigenvalues --    0.36632   0.37090   0.37292   0.38879
0.39471
 Alpha virt. eigenvalues --    0.40087   0.40311   0.40871   0.41911
0.42720
 Alpha virt. eigenvalues --    0.43397   0.43635   0.44803   0.44906
0.45277
 Alpha virt. eigenvalues --    0.45959   0.47439   0.51348   0.52255
0.55101
 Alpha virt. eigenvalues --    0.56622   0.57206   0.59348   0.61948
0.62748
 Alpha virt. eigenvalues --    0.65282   0.65981   0.67800   0.68755
0.68866
 Alpha virt. eigenvalues --    0.69516   0.70648   0.70919   0.71659
0.72280
 Alpha virt. eigenvalues --    0.72548   0.73467   0.73778   0.74288
0.74895
 Alpha virt. eigenvalues --    0.75228   0.75444   0.76264   0.77411
0.78174
 Alpha virt. eigenvalues --    0.79337   0.79474   0.80187   0.80558
0.81497
 Alpha virt. eigenvalues --    0.82007   0.82805   0.83298   0.85059
0.86159
 Alpha virt. eigenvalues --    0.86802   0.87594   0.88518   0.89067
0.89697
 Alpha virt. eigenvalues --    0.90525   0.90932   0.91514   0.92314
0.92514
 Alpha virt. eigenvalues --    0.93588   0.93995   0.94302   0.95373
0.95988
 Alpha virt. eigenvalues --    0.96664   0.97768   0.99423   1.00508
1.01953
 Alpha virt. eigenvalues --    1.02426   1.03126   1.04421   1.05734
1.07073
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    1.07227   1.07421   1.08478   1.09975
1.10513
 Alpha virt. eigenvalues --    1.11568   1.12649   1.14266   1.15220
1.15909
 Alpha virt. eigenvalues --    1.16633   1.18530   1.19882   1.20714
1.20843
 Alpha virt. eigenvalues --    1.21266   1.22921   1.24512   1.24776
1.25529
 Alpha virt. eigenvalues --    1.27219   1.27963   1.28197   1.28799
1.30118
 Alpha virt. eigenvalues --    1.31752   1.32721   1.33789   1.35110
1.36292
 Alpha virt. eigenvalues --    1.36546   1.38608   1.38809   1.39804
1.40625
 Alpha virt. eigenvalues --    1.41328   1.42211   1.42788   1.43462
1.44360
 Alpha virt. eigenvalues --    1.44660   1.45025   1.46147   1.46481
1.46774
 Alpha virt. eigenvalues --    1.47456   1.48959   1.49321   1.50512
1.51383
 Alpha virt. eigenvalues --    1.52965   1.54767   1.55040   1.57243
1.59301
 Alpha virt. eigenvalues --    1.61379   1.64239   1.65860   1.67204
1.68034
 Alpha virt. eigenvalues --    1.71927   1.72859   1.75400   1.76868
1.78389
 Alpha virt. eigenvalues --    1.80389   1.81230   1.81424   1.82731
1.83012
 Alpha virt. eigenvalues --    1.83438   1.85640   1.85862   1.86926
1.87229
 Alpha virt. eigenvalues --    1.88481   1.89417   1.91401   1.91915
1.92072
 Alpha virt. eigenvalues --    1.92568   1.93573   1.94659   1.95238
1.97030
 Alpha virt. eigenvalues --    1.97432   1.97846   1.98669   1.99915
2.01106
 Alpha virt. eigenvalues --    2.02822   2.03698   2.05706   2.06706
2.07555
 Alpha virt. eigenvalues --    2.08579   2.09822   2.10931   2.12510
2.12730
 Alpha virt. eigenvalues --    2.14705   2.17914   2.18588   2.18876
2.19382
 Alpha virt. eigenvalues --    2.20766   2.22339   2.24559   2.24931
2.26426
 Alpha virt. eigenvalues --    2.27402   2.27964   2.28716   2.31026
2.31722
 Alpha virt. eigenvalues --    2.32079   2.32815   2.34664   2.36159
2.40369
 Alpha virt. eigenvalues --    2.41217   2.41469   2.47473   2.49148
2.49928
 Alpha virt. eigenvalues --    2.55282   2.59428   2.59627   2.60003
2.61832
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    2.62262   2.64827   2.65910   2.67667
2.68842
 Alpha virt. eigenvalues --    2.69813   2.72063   2.73603   2.75028
2.75393
 Alpha virt. eigenvalues --    2.76977   2.81298   2.82878   2.83212
2.84270
 Alpha virt. eigenvalues --    2.85521   2.86506   2.90185   2.93379
2.94357
 Alpha virt. eigenvalues --    2.94982   2.97329   3.09111   3.11273
3.13787
 Alpha virt. eigenvalues --    3.17421   3.18515   3.23163   3.24169
3.32083
 Alpha virt. eigenvalues --    3.34509   3.40363   3.46438   4.23745
4.28669
 Alpha virt. eigenvalues --    4.31077   4.31598   4.33624   4.36133
4.37505
 Alpha virt. eigenvalues --    4.38613   4.41124   4.43716   4.46248
4.47382
 Alpha virt. eigenvalues --    4.50754   4.51972   4.53038   4.59012
4.64732
 Alpha virt. eigenvalues --    4.68718   4.70577   4.74572   4.85104
5.00795
 Alpha virt. eigenvalues --    5.33136
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   45.151332 -15.297888  11.983425 -21.254271   0.053028
0.979161
     2  C  -15.297888  29.076801  -8.365286  17.542849  -0.015978  -
1.569637
     3  C   11.983425  -8.365286  23.810990 -16.630865   0.001969
1.048978
     4  C  -21.254271  17.542849 -16.630865  43.946578   0.164898  -
1.539958
     5  H    0.053028  -0.015978   0.001969   0.164898   0.519064
0.004928
     6  C    0.979161  -1.569637   1.048978  -1.539958   0.004928
9.561269
     7  H    0.019518  -0.011907   0.005605  -0.063070  -0.001217
0.359392
     8  C   -0.384748   0.384222  -0.056970  -0.210069   0.015758  -
2.297721
     9  H   -0.005684   0.023008   0.024804   0.004231  -0.000030
0.002319
    10  C  -16.005122   3.789771  -3.936176   3.965019  -0.005324  -
0.006036
    11  H   -0.046992  -0.071243   0.073122   0.010553   0.000002
0.003130
    12  C    0.772337  -1.613509   1.663639  -0.393103   0.004275  -
0.144339
    13  H    0.001857  -0.008278   0.013462   0.002723   0.000000
0.001627
```

This journal is © The Royal Society of Chemistry 2014

14	C	-1.239219	0.587960	-2.659620	0.896535	0.006181	0.099923
15	H	0.026616	0.010414	0.006023	-0.019051	-0.000006	-0.001660
16	C	-7.861309	2.244013	-7.064564	6.658641	0.005565	-0.028803
17	H	0.067918	0.016959	-0.050564	-0.027302	0.003762	-0.009591
18	C	7.402933	-8.616059	6.680989	-16.543062	0.025631	0.592311
19	C	7.138496	-12.875825	4.271272	-17.675443	0.032761	1.255523
20	C	1.032232	0.268868	-0.340647	0.179332	0.009296	-0.271983
21	H	0.017336	-0.028468	-0.002037	-0.007176	0.000002	-0.001493
22	C	-0.300762	-0.261066	-0.057946	0.380009	-0.001728	-0.036609
23	H	-0.002515	-0.001681	0.000513	0.003665	0.000000	-0.000033
24	C	-0.061139	-0.100757	-0.242161	-0.204669	-0.004230	0.056408
25	H	0.000658	0.005860	-0.002492	-0.002976	-0.000006	-0.000246
26	C	-2.046153	0.153430	-0.760639	3.490921	-0.015023	-0.127067
27	H	0.001330	0.004677	-0.006235	-0.030956	0.003567	0.002679
28	C	0.108319	0.422616	-0.309595	0.151371	0.000763	0.955611
29	C	-1.181346	1.166473	-0.899593	2.171146	-0.030271	-1.746264
30	O	-0.040664	0.034976	-0.106963	0.128101	0.000118	-0.392794
31	O	0.084036	-0.056445	0.187067	-0.210646	0.004249	-0.043009
32	O	0.188052	-0.099557	0.021568	-0.069850	0.000024	-0.052654
33	C	-3.823493	-0.573838	-2.172110	0.475578	0.005277	-0.520287
34	N	0.040961	0.110183	0.113983	0.045681	-0.000015	0.021787

		7	8	9	10	11	12
1	C	0.019518	-0.384748	-0.005684	-16.005122	-0.046992	0.772337
2	C	-0.011907	0.384222	0.023008	3.789771	-0.071243	-1.613509
3	C	0.005605	-0.056970	0.024804	-3.936176	0.073122	1.663639
4	C	-0.063070	-0.210069	0.004231	3.965019	0.010553	-0.393103

This journal is © The Royal Society of Chemistry 2014

5	H	-0.001217	0.015758	-0.000030	-0.005324	0.000002	0.004275
6	C	0.359392	-2.297721	0.002319	-0.006036	0.003130	-0.144339
7	H	0.464283	-0.006039	-0.001861	-0.004344	0.000000	0.000267
8	C	-0.006039	9.792606	0.330849	0.824896	-0.011499	0.309499
9	H	-0.001861	0.330849	0.459866	0.019190	-0.000003	-0.000581
10	C	-0.004344	0.824896	0.019190	20.269304	0.274616	-2.477037
11	H	0.000000	-0.011499	-0.000003	0.274616	0.501538	0.124828
12	C	0.000267	0.309499	-0.000581	-2.477037	0.124828	9.622842
13	H	0.000000	-0.002642	0.000000	0.030806	-0.003997	0.281597
14	C	-0.000382	-0.013302	0.001217	0.334656	0.007035	0.736893
15	H	0.000000	0.001126	0.000000	0.027397	-0.000153	-0.052224
16	C	0.003051	0.402259	0.000207	5.240544	-0.013110	-1.360428
17	H	0.000001	0.004825	0.000000	-0.025862	0.000015	0.004132
18	C	0.049026	-0.468565	-0.000970	-2.586070	-0.005346	-0.186705
19	C	0.025196	-1.119201	0.056040	-1.382608	-0.028949	-0.276575
20	C	0.003648	-0.183566	-0.058516	-1.909654	-0.002827	-0.018066
21	H	0.000000	-0.001070	-0.000051	-0.004122	0.000001	0.000067
22	C	0.001393	0.114660	-0.011789	0.211731	-0.000491	-0.010992
23	H	0.000000	0.000026	0.000000	0.000200	0.000000	0.000009
24	C	-0.009368	-0.170071	-0.003085	-0.173269	-0.000047	-0.018732
25	H	0.000001	0.000064	0.000000	-0.000123	0.000000	0.000005
26	C	-0.027510	-0.244380	-0.002252	-0.583141	-0.000352	-0.089217
27	H	-0.000017	-0.000920	0.000000	0.000297	0.000000	-0.000090
28	C	0.010055	-2.003415	-0.072257	-0.589129	0.012323	-0.221015
29	C	-0.079935	0.962709	0.015349	0.186241	-0.002605	0.113009
30	O	0.008211	-0.222212	0.008256	-0.030079	0.000091	0.019595

This journal is © The Royal Society of Chemistry 2014

31	O	0.001478	-0.074734	-0.000590	-0.016776	-0.000001	-0.007268
32	O	-0.000599	-0.093649	0.003331	-0.082347	-0.000055	-0.027261
33	C	0.003814	0.268375	-0.053641	1.187442	-0.050574	-0.373814
34	N	-0.000141	0.020955	0.001850	0.061610	0.012076	0.064450

		13	14	15	16	17	18
1	C	0.001857	-1.239219	0.026616	-7.861309	0.067918	7.402933
2	C	-0.008278	0.587960	0.010414	2.244013	0.016959	-8.616059
3	C	0.013462	-2.659620	0.006023	-7.064564	-0.050564	6.680989
4	C	0.002723	0.896535	-0.019051	6.658641	-0.027302	-16.543062
5	H	0.000000	0.006181	-0.000006	0.005565	0.003762	0.025631
6	C	0.001627	0.099923	-0.001660	-0.028803	-0.009591	0.592311
7	H	0.000000	-0.000382	0.000000	0.003051	0.000001	0.049026
8	C	-0.002642	-0.013302	0.001126	0.402259	0.004825	-0.468565
9	H	0.000000	0.001217	0.000000	0.000207	0.000000	-0.000970
10	C	0.030806	0.334656	0.027397	5.240544	-0.025862	-2.586070
11	H	-0.003997	0.007035	-0.000153	-0.013110	0.000015	-0.005346
12	C	0.281597	0.736893	-0.052224	-1.360428	0.004132	-0.186705
13	H	0.514378	-0.040629	-0.004143	0.018316	-0.000156	0.002193
14	C	-0.040629	7.354110	0.293404	1.379296	0.075552	-0.831179
15	H	-0.004143	0.293404	0.517739	0.002628	-0.004328	-0.002010
16	C	0.018316	1.379296	0.002628	12.428456	0.257120	-2.604652
17	H	-0.000156	0.075552	-0.004328	0.257120	0.525773	-0.035969
18	C	0.002193	-0.831179	-0.002010	-2.604652	-0.035969	21.636183
19	C	-0.001437	-0.420172	0.002294	-2.633431	-0.005309	10.015319
20	C	0.000165	-0.092949	-0.000214	-0.632609	0.000270	-0.597995
21	H	0.000000	-0.000100	0.000000	-0.000238	0.000000	0.027500

This journal is © The Royal Society of Chemistry 2014

22	C	0.000002	0.015411	0.000015	0.108062	-0.000076	0.430478
23	H	0.000000	0.000005	0.000000	-0.000094	0.000000	0.006671
24	C	0.000016	-0.022884	-0.000007	-0.156184	-0.000199	-1.636310
25	H	0.000000	-0.000002	0.000000	0.000154	0.000000	0.017727
26	C	-0.000107	-0.102293	0.000052	-0.499374	0.000730	-3.621614
27	H	0.000000	0.000543	0.000000	0.002683	0.000001	-0.025318
28	C	0.004107	-0.014019	-0.001637	-0.273615	-0.002776	0.168519
29	C	-0.002046	-0.033153	0.002875	0.236188	0.007926	-0.861102
30	O	-0.000029	0.023988	-0.000011	0.003270	0.000244	-0.041553
31	O	0.000001	-0.040321	-0.000080	-0.094671	0.000019	0.071056
32	O	-0.000114	-0.003176	-0.000001	0.000470	-0.000001	0.024988
33	C	-0.003629	0.018439	0.001149	0.134708	0.001109	-2.158695
34	N	0.000010	0.006261	-0.000008	0.013824	0.000002	0.029421

		19	20	21	22	23	24
1	C	7.138496	1.032232	0.017336	-0.300762	-0.002515	-0.061139
2	C	-12.875825	0.268868	-0.028468	-0.261066	-0.001681	-0.100757
3	C	4.271272	-0.340647	-0.002037	-0.057946	0.000513	-0.242161
4	C	-17.675443	0.179332	-0.007176	0.380009	0.003665	-0.204669
5	H	0.032761	0.009296	0.000002	-0.001728	0.000000	-0.004230
6	C	1.255523	-0.271983	-0.001493	-0.036609	-0.000033	0.056408
7	H	0.025196	0.003648	0.000000	0.001393	0.000000	-0.009368
8	C	-1.119201	-0.183566	-0.001070	0.114660	0.000026	-0.170071
9	H	0.056040	-0.058516	-0.000051	-0.011789	0.000000	-0.003085
10	C	-1.382608	-1.909654	-0.004122	0.211731	0.000200	-0.173269
11	H	-0.028949	-0.002827	0.000001	-0.000491	0.000000	-0.000047
12	C	-0.276575	-0.018066	0.000067	-0.010992	0.000009	-0.018732

This journal is © The Royal Society of Chemistry 2014

13	H	-0.001437	0.000165	0.000000	0.000002	0.000000	0.000016
14	C	-0.420172	-0.092949	-0.000100	0.015411	0.000005	-0.022884
15	H	0.002294	-0.000214	0.000000	0.000015	0.000000	-0.000007
16	C	-2.633431	-0.632609	-0.000238	0.108062	-0.000094	-0.156184
17	H	-0.005309	0.000270	0.000000	-0.000076	0.000000	-0.000199
18	C	10.015319	-0.597995	0.027500	0.430478	0.006671	-1.636310
19	C	36.150501	-10.932011	-0.094512	1.325434	-0.004030	-0.455798
20	C	-10.932011	18.408344	0.313741	-2.877553	0.023130	0.550575
21	H	-0.094512	0.313741	0.499290	0.072781	-0.003913	0.020498
22	C	1.325434	-2.877553	0.072781	7.662619	0.304518	0.417485
23	H	-0.004030	0.023130	-0.003913	0.304518	0.514213	-0.037970
24	C	-0.455798	0.550575	0.020498	0.417485	-0.037970	7.151632
25	H	0.005601	0.008993	-0.000149	-0.035748	-0.004048	0.301037
26	C	-5.182022	3.934422	-0.014488	-1.291444	0.009401	1.083364
27	H	0.066377	-0.026941	0.000015	0.003294	-0.000153	0.026710
28	C	0.371836	0.231927	0.004218	0.062036	0.000114	0.011314
29	C	-1.015528	-0.050082	-0.001090	-0.021411	-0.000053	0.078040
30	O	-0.052826	0.012849	0.000001	-0.002885	0.000000	0.002799
31	O	0.043123	0.003166	0.000000	-0.000173	0.000000	-0.000286
32	O	-0.005808	0.007287	-0.000030	-0.003488	0.000000	0.000487
33	C	-0.724355	-0.691439	-0.018276	0.207413	-0.003245	-0.138346
34	N	-0.287847	0.031879	0.005516	0.013997	0.000074	0.000840

		25	26	27	28	29	30
1	C	0.000658	-2.046153	0.001330	0.108319	-1.181346	-0.040664
2	C	0.005860	0.153430	0.004677	0.422616	1.166473	0.034976
3	C	-0.002492	-0.760639	-0.006235	-0.309595	-0.899593	-0.106963

This journal is © The Royal Society of Chemistry 2014

```
     4  C   -0.002976   3.490921  -0.030956   0.151371   2.171146
0.128101
     5  H   -0.000006  -0.015023   0.003567   0.000763  -0.030271
0.000118
     6  C   -0.000246  -0.127067   0.002679   0.955611  -1.746264  -
0.392794
     7  H    0.000001  -0.027510  -0.000017   0.010055  -0.079935
0.008211
     8  C    0.000064  -0.244380  -0.000920  -2.003415   0.962709  -
0.222212
     9  H    0.000000  -0.002252   0.000000  -0.072257   0.015349
0.008256
    10  C   -0.000123  -0.583141   0.000297  -0.589129   0.186241  -
0.030079
    11  H    0.000000  -0.000352   0.000000   0.012323  -0.002605
0.000091
    12  C    0.000005  -0.089217  -0.000090  -0.221015   0.113009
0.019595
    13  H    0.000000  -0.000107   0.000000   0.004107  -0.002046  -
0.000029
    14  C   -0.000002  -0.102293   0.000543  -0.014019  -0.033153
0.023988
    15  H    0.000000   0.000052   0.000000  -0.001637   0.002875  -
0.000011
    16  C    0.000154  -0.499374   0.002683  -0.273615   0.236188
0.003270
    17  H    0.000000   0.000730   0.000001  -0.002776   0.007926
0.000244
    18  C    0.017727  -3.621614  -0.025318   0.168519  -0.861102  -
0.041553
    19  C    0.005601  -5.182022   0.066377   0.371836  -1.015528  -
0.052826
    20  C    0.008993   3.934422  -0.026941   0.231927  -0.050082
0.012849
    21  H   -0.000149  -0.014488   0.000015   0.004218  -0.001090
0.000001
    22  C   -0.035748  -1.291444   0.003294   0.062036  -0.021411  -
0.002885
    23  H   -0.004048   0.009401  -0.000153   0.000114  -0.000053
0.000000
    24  C    0.301037   1.083364   0.026710   0.011314   0.078040
0.002799
    25  H    0.517967  -0.001732  -0.004274  -0.000080   0.000123
0.000000
    26  C   -0.001732  11.357802   0.262610   0.070704   0.110757
0.027749
    27  H   -0.004274   0.262610   0.527836  -0.000659   0.002066
0.000002
    28  C   -0.000080   0.070704  -0.000659   7.129571  -1.110845
0.281386
    29  C    0.000123   0.110757   0.002066  -1.110845   6.950657
0.318463
```

This journal is © The Royal Society of Chemistry 2014

```
    30  O    0.000000   0.027749   0.000002   0.281386   0.318463
8.307724
    31  O    0.000000   0.013445   0.000007   0.036494   0.420917  -
0.080808
    32  O    0.000000   0.000199   0.000000   0.472733   0.022553  -
0.070992
    33  C    0.000757  -0.275698   0.000948   0.071096   0.036878
0.054093
    34  N   -0.000001   0.003943  -0.000001  -0.049162   0.003105  -
0.001438
              31         32         33         34
     1  C    0.084036   0.188052  -3.823493   0.040961
     2  C   -0.056445  -0.099557  -0.573838   0.110183
     3  C    0.187067   0.021568  -2.172110   0.113983
     4  C   -0.210646  -0.069850   0.475578   0.045681
     5  H    0.004249   0.000024   0.005277  -0.000015
     6  C   -0.043009  -0.052654  -0.520287   0.021787
     7  H    0.001478  -0.000599   0.003814  -0.000141
     8  C   -0.074734  -0.093649   0.268375   0.020955
     9  H   -0.000590   0.003331  -0.053641   0.001850
    10  C   -0.016776  -0.082347   1.187442   0.061610
    11  H   -0.000001  -0.000055  -0.050574   0.012076
    12  C   -0.007268  -0.027261  -0.373814   0.064450
    13  H    0.000001  -0.000114  -0.003629   0.000010
    14  C   -0.040321  -0.003176   0.018439   0.006261
    15  H   -0.000080  -0.000001   0.001149  -0.000008
    16  C   -0.094671   0.000470   0.134708   0.013824
    17  H    0.000019  -0.000001   0.001109   0.000002
    18  C    0.071056   0.024988  -2.158695   0.029421
    19  C    0.043123  -0.005808  -0.724355  -0.287847
    20  C    0.003166   0.007287  -0.691439   0.031879
    21  H    0.000000  -0.000030  -0.018276   0.005516
    22  C   -0.000173  -0.003488   0.207413   0.013997
    23  H    0.000000   0.000000  -0.003245   0.000074
    24  C   -0.000286   0.000487  -0.138346   0.000840
    25  H    0.000000   0.000000   0.000757  -0.000001
    26  C    0.013445   0.000199  -0.275698   0.003943
    27  H    0.000007   0.000000   0.000948  -0.000001
    28  C    0.036494   0.472733   0.071096  -0.049162
    29  C    0.420917   0.022553   0.036878   0.003105
    30  O   -0.080808  -0.070992   0.054093  -0.001438
    31  O    8.144928   0.000312  -0.000002  -0.000033
    32  O    0.000312   8.070519   0.034120  -0.004722
    33  C   -0.000002   0.034120  15.023431   0.134180
    34  N   -0.000033  -0.004722   0.134180   6.965252
 Mulliken atomic charges:
              1
     1  C    0.481758
     2  C   -0.275659
     3  C   -0.242948
     4  C    0.664637
     5  H    0.212711
```

This journal is © The Royal Society of Chemistry 2014

```
     6  C   -0.154863
     7  H    0.251450
     8  C    0.131943
     9  H    0.260793
    10  C   -0.606501
    11  H    0.218912
    12  C   -0.446491
    13  H    0.195946
    14  C   -0.324009
    15  H    0.193803
    16  C    0.083629
    17  H    0.195776
    18  C   -0.357770
    19  C    0.413913
    20  C   -0.333073
    21  H    0.216245
    22  C   -0.417179
    23  H    0.195195
    24  C   -0.265694
    25  H    0.192930
    26  C    0.364977
    27  H    0.189921
    28  C    0.071093
    29  C    0.229851
    30  O   -0.188662
    31  O   -0.384458
    32  O   -0.332336
    33  C   -0.077364
    34  N   -0.358475
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
              1
     1  C    0.481758
     2  C   -0.275659
     3  C   -0.242948
     4  C    0.877348
     5  H    0.000000
     6  C    0.096587
     7  H    0.000000
     8  C    0.392736
     9  H    0.000000
    10  C   -0.387589
    11  H    0.000000
    12  C   -0.250544
    13  H    0.000000
    14  C   -0.130206
    15  H    0.000000
    16  C    0.279405
    17  H    0.000000
    18  C   -0.357770
    19  C    0.413913
    20  C   -0.116828
```

This journal is © The Royal Society of Chemistry 2014

```
   21  H    0.000000
   22  C   -0.221985
   23  H    0.000000
   24  C   -0.072765
   25  H    0.000000
   26  C    0.554898
   27  H    0.000000
   28  C    0.071093
   29  C    0.229851
   30  O   -0.188662
   31  O   -0.384458
   32  O   -0.332336
   33  C   -0.077364
   34  N   -0.358475
Sum of Mulliken charges=   0.00000
APT atomic charges:
             1
    1  C   -0.089365
    2  C    0.386404
    3  C   -0.096725
    4  C    0.333490
    5  H    0.012750
    6  C   -0.269811
    7  H    0.042537
    8  C   -0.199328
    9  H    0.045778
   10  C   -0.030884
   11  H    0.060254
   12  C   -0.001805
   13  H    0.037404
   14  C   -0.017091
   15  H    0.035065
   16  C   -0.000208
   17  H    0.040220
   18  C   -0.086990
   19  C   -0.078642
   20  C   -0.034896
   21  H    0.057568
   22  C   -0.017468
   23  H    0.034986
   24  C   -0.032994
   25  H    0.032536
   26  C   -0.004572
   27  H    0.034956
   28  C    1.042240
   29  C    1.103902
   30  O   -0.736245
   31  O   -0.725410
   32  O   -0.657413
   33  C    0.037274
   34  N   -0.257515
Sum of APT charges=   0.00000
```

This journal is © The Royal Society of Chemistry 2014

```
APT Atomic charges with hydrogens summed into heavy atoms:
              1
    1  C   -0.089365
    2  C    0.386404
    3  C   -0.096725
    4  C    0.346240
    5  H    0.000000
    6  C   -0.227274
    7  H    0.000000
    8  C   -0.153550
    9  H    0.000000
   10  C    0.029370
   11  H    0.000000
   12  C    0.035598
   13  H    0.000000
   14  C    0.017974
   15  H    0.000000
   16  C    0.040012
   17  H    0.000000
   18  C   -0.086990
   19  C   -0.078642
   20  C    0.022672
   21  H    0.000000
   22  C    0.017518
   23  H    0.000000
   24  C   -0.000458
   25  H    0.000000
   26  C    0.030384
   27  H    0.000000
   28  C    1.042240
   29  C    1.103902
   30  O   -0.736245
   31  O   -0.725410
   32  O   -0.657413
   33  C    0.037274
   34  N   -0.257515
Sum of APT charges=   0.00000
Electronic spatial extent (au):  <R**2>=  5281.1187
Charge=     0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=     4.8553    Y=    -4.0321    Z=     3.0041  Tot=     6.9897
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=  -123.9590   YY=  -148.1174   ZZ=  -132.3878
  XY=    -6.3242   XZ=   -15.8352   YZ=     0.8375
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=    10.8624   YY=   -13.2960   ZZ=     2.4336
  XY=    -6.3242   XZ=   -15.8352   YZ=     0.8375
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=    52.3856  YYY=   -82.6136  ZZZ=   -27.5802  XYY=    18.1855
 XXY=     3.0037  XXZ=    36.6450  XZZ=   -18.3072  YZZ=    -4.8453
 YYZ=    32.6768  XYZ=     0.5755
Hexadecapole moment (field-independent basis, Debye-Ang**3):
```

This journal is © The Royal Society of Chemistry 2014

```
 XXXX= -3302.9015 YYYY= -2375.1093 ZZZZ= -1579.3640 XXXY=   -40.0622
 XXXZ=  -120.5920 YYYX=  -107.2424 YYYZ=    -5.7307 ZZZX=   -27.0775
 ZZZY=    14.5637 XXYY=  -939.0664 XXZZ=  -877.9546 YYZZ=  -627.9235
 XXYZ=   -13.1538 YYXZ=   -64.7803 ZZXY=    10.8807
 N-N= 1.867282541538D+03 E-N=-6.082759817952D+03  KE=
1.001618819125D+03
  Exact polarizability: 293.074  -2.521 244.784 -18.351  -4.147
183.384
 Approx polarizability: 465.425  -0.765 482.681 -29.373 -13.366
310.486
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.007170665    0.005103847   -0.001926754
    2          6          -0.002573544   -0.006168113   -0.047109468
    3          6           0.002041574   -0.001672291   -0.000597216
    4          6           0.000547414    0.001633179   -0.000373979
    5          1          -0.000179809   -0.000461833   -0.000166934
    6          6           0.000048817   -0.000997470   -0.002004045
    7          1           0.000385571    0.000255865   -0.000120928
    8          6           0.000615205   -0.004965251    0.003945615
    9          1           0.000256397    0.000445263   -0.000135461
   10          6          -0.000445755    0.000409294   -0.000598240
   11          1          -0.000204314    0.000246116    0.000730212
   12          6           0.000518473   -0.000331828    0.001094460
   13          1           0.000297868   -0.000142960   -0.000095622
   14          6          -0.000070402    0.000061760    0.000035949
   15          1           0.000133309   -0.000061953    0.000009426
   16          6          -0.000329051    0.000055771   -0.000403796
   17          1           0.000217490   -0.000083011   -0.000187147
   18          6          -0.002547522   -0.000093734   -0.000986030
   19          6           0.008810783    0.000031487   -0.001840580
   20          6           0.000810324    0.000108935   -0.000871544
   21          1           0.000203151    0.000094832    0.000895713
   22          6          -0.000795713    0.000018689    0.001110948
   23          1          -0.000356465    0.000042262   -0.000109701
   24          6           0.000016036    0.000018827    0.000085712
   25          1          -0.000153723    0.000037407    0.000028616
   26          6           0.000413420   -0.000064073   -0.000449054
   27          1          -0.000247423    0.000042083   -0.000221484
   28          6          -0.005047679   -0.000843692   -0.004456098
   29          6          -0.002940213    0.000051682    0.000221738
   30          8           0.001114479    0.000266143    0.001707838
   31          8           0.001144701    0.000139089   -0.000768445
   32          8           0.001729028   -0.000264459    0.004386434
   33          6           0.003929784    0.010405624    0.087077120
   34          7          -0.000171548   -0.003317485   -0.037907256
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.087077120 RMS     0.010726576
```

This journal is © The Royal Society of Chemistry 2014

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.047832573 RMS     0.004720981
 Search for a saddle point.
 Step number   1 out of a maximum of 195
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Second derivative matrix not updated -- analytic derivatives used.
     Eigenvalues ---   -0.01975   0.00285   0.00742   0.00789
0.01144
     Eigenvalues ---    0.01224   0.01480   0.01543   0.01605
0.01646
     Eigenvalues ---    0.01746   0.01809   0.01909   0.01919
0.01949
     Eigenvalues ---    0.02016   0.02108   0.02166   0.02223
0.02277
     Eigenvalues ---    0.02399   0.02475   0.02492   0.02511
0.02714
     Eigenvalues ---    0.02759   0.02771   0.02778   0.03438
0.04048
     Eigenvalues ---    0.05470   0.06601   0.07010   0.07540
0.08524
     Eigenvalues ---    0.10392   0.11118   0.11162   0.11193
0.11822
     Eigenvalues ---    0.11894   0.12501   0.12521   0.12651
0.12701
     Eigenvalues ---    0.12935   0.14251   0.16210   0.16501
0.17591
     Eigenvalues ---    0.18914   0.19179   0.19183   0.19396
0.19446
     Eigenvalues ---    0.19735   0.19789   0.20958   0.21966
0.23793
     Eigenvalues ---    0.24015   0.25136   0.25611   0.27749
0.28465
     Eigenvalues ---    0.29502   0.30080   0.30817   0.31516
0.33448
     Eigenvalues ---    0.34194   0.35305   0.35876   0.35904
0.36041
     Eigenvalues ---    0.36125   0.36226   0.36265   0.36292
0.36350
     Eigenvalues ---    0.37236   0.38023   0.39091   0.40151
0.40793
     Eigenvalues ---    0.41732   0.42420   0.42900   0.44738
0.47342
     Eigenvalues ---    0.47622   0.50295   0.50637   0.88539
0.89747
     Eigenvalues ---
1.374751000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
         1             -0.05213   0.02379   0.17531   0.01836
0.44611
                           R6        R7        R8        R9        R10
         1              0.15818  -0.05269  -0.02055  -0.05389
0.16214
                           R11       R12       R13       R14       R15
         1              0.01851  -0.00854   0.39078   0.14886  -
0.05405
                           R16       R17       R18       R19       R20
         1              0.25610  -0.00652  -0.09543   0.16161  -
0.00565
                           R21       R22       R23       R24       R25
         1             -0.03404  -0.00911   0.18422  -0.01252  -
0.03356
                           R26       R27       R28       R29       R30
         1              0.06433  -0.00034  -0.01448   0.00003
0.01605
                           R31       R32       R33       R34       R35
```

This journal is © The Royal Society of Chemistry 2014

1	-0.00017	-0.01521	-0.00026	0.02036	0.01788

	R36	R37	R38	R39	R40
1	0.01828	-0.00031	-0.01415	0.00004	0.01556

	R41	R42	R43	R44	R45
1	-0.00010	-0.01476	-0.00012	0.00353	0.00197

	R46	R47	R48	A1	A2
1	-0.00399	0.00210	0.00134	0.02039	-0.01031

	A3	A4	A5	A6	A7
1	-0.00897	0.04705	0.02303	0.01801	0.01847

	A8	A9	A10	A11	A12
1	-0.00472	-0.01297	0.02149	0.04792	0.01850

	A13	A14	A15	A16	A17
1	0.04902	0.02885	0.01304	0.05853	0.01659

	A18	A19	A20	A21	A22
1	0.02767	-0.00555	0.00516	0.00038	-0.00003

	A23	A24	A25	A26	A27
1	0.00338	-0.00334	-0.00231	0.00068	0.00164

	A28	A29	A30	A31	A32
1	0.00455	-0.00620	0.00164	0.01871	-0.01392

	A33	A34	A35	A36	A37
1	-0.00414	0.02157	-0.01156	-0.00883	-0.00553

	A38	A39	A40	A41	A42
1	0.00536	0.00013	0.00032	0.00277	-0.00309

	A43	A44	A45	A46	A47
1	-0.00222	0.00038	0.00185	0.00450	-0.00602

	A48	A49	A50	A51	A52
1	0.00148	-0.00466	0.00513	-0.00044	-0.00381

	A53	A54	A55	A56	A57
1	0.00047	0.00337	-0.01378	0.00177	0.01119

	D1	D2	D3	D4	D5
1	0.16597	-0.03512	0.15124	-0.04985	-0.00334

	D6	D7	D8	D9	D10
1	-0.01271	0.01058	0.00122	0.01254	0.01419

	D11	D12	D13	D14	D15

```
          1             -0.00396  -0.00232  -0.16662  -0.15170
0.03660
                           D16       D17       D18       D19       D20
          1              0.05152   0.04395  -0.15689   0.05426  -
0.14657
                           D21       D22       D23       D24       D25
          1              0.00048   0.00258  -0.01119  -0.00910
0.15570
                           D26       D27       D28       D29       D30
          1              0.14743  -0.04672  -0.05499  -0.01372
0.17020
                           D31       D32       D33       D34       D35
          1             -0.17797   0.00595  -0.13845  -0.14169
0.02152
                           D36       D37       D38       D39       D40
          1              0.01827  -0.03175  -0.02784   0.15040
0.15432
                           D41       D42       D43       D44       D45
          1             -0.00002   0.00149   0.00167   0.00318  -
0.00124
                           D46       D47       D48       D49       D50
          1              0.00003   0.00029   0.00156  -0.00097  -
0.00313
                           D51       D52       D53       D54       D55
          1              0.00027  -0.00188   0.00517  -0.00883
0.01246
                           D56       D57       D58       D59       D60
          1             -0.00155   0.00997   0.00682   0.00038  -
0.00277
                           D61       D62       D63       D64       D65
          1             -0.01190  -0.01495   0.00492   0.00187
0.00124
                           D66       D67       D68       D69       D70
          1             -0.00084  -0.00190  -0.00398   0.00175  -
0.00019
                           D71       D72       D73       D74       D75
          1             -0.00033  -0.00227   0.00039   0.00365  -
0.00155
                           D76       D77       D78       D79       D80
          1              0.00171   0.04811   0.04458  -0.04441  -
0.04152
 RFO step:  Lambda0=4.051730575D-04 Lambda=-1.49393281D-02.
 Linear search not attempted -- option 19 set.
 Maximum step size (   0.300) exceeded in Quadratic search.
    -- Step size scaled by   0.893
 Iteration  1 RMS(Cart)=  0.03697645 RMS(Int)=  0.00143731
 Iteration  2 RMS(Cart)=  0.00195547 RMS(Int)=  0.00006556
 Iteration  3 RMS(Cart)=  0.00000453 RMS(Int)=  0.00006552
 Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00006552
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
```

This journal is © The Royal Society of Chemistry 2014

R1	2.71835	0.00457	0.00000	0.02854	0.02856
2.74692					
R2	2.68910	0.00058	0.00000	-0.00495	-0.00499
2.68411					
R3	5.31147	0.00224	0.00000	0.00784	0.00780
5.31927					
R4	2.67135	0.00002	0.00000	-0.00421	-0.00421
2.66713					
R5	4.18566	0.00662	0.00000	0.01128	0.01133
4.19698					
R6	4.72187	0.00097	0.00000	-0.00059	-0.00070
4.72117					
R7	2.72439	0.00401	0.00000	0.02842	0.02842
2.75281					
R8	2.91018	-0.04783	0.00000	-0.21656	-0.21662
2.69356					
R9	2.71836	-0.00058	0.00000	0.00506	0.00504
2.72340					
R10	5.31148	0.00049	0.00000	-0.02975	-0.02978
5.28170					
R11	2.67135	-0.00034	0.00000	-0.00286	-0.00287
2.66848					
R12	2.05710	0.00188	0.00000	0.00138	0.00131
2.05841					
R13	4.18567	-0.00184	0.00000	-0.09787	-0.09789
4.08778					
R14	4.72187	0.00130	0.00000	-0.03735	-0.03735
4.68453					
R15	2.72439	-0.00074	0.00000	0.00506	0.00507
2.72947					
R16	5.02859	-0.00345	0.00000	-0.09577	-0.09565
4.93295					
R17	2.04439	-0.00046	0.00000	0.00168	0.00168
2.04606					
R18	2.66751	-0.00399	0.00000	0.00568	0.00579
2.67330					
R19	5.13945	-0.00020	0.00000	-0.04487	-0.04496
5.09448					
R20	2.79858	0.00055	0.00000	0.00670	0.00672
2.80530					
R21	5.18928	-0.00018	0.00000	-0.02317	-0.02316
5.16612					
R22	2.04438	0.00015	0.00000	-0.00011	-0.00007
2.04432					
R23	5.13944	0.00452	0.00000	0.03636	0.03639
5.17583					
R24	2.79858	0.00348	0.00000	0.00782	0.00782
2.80640					
R25	5.18928	-0.00081	0.00000	0.04841	0.04840
5.23768					
R26	5.36130	-0.00388	0.00000	-0.03848	-0.03837
5.32293					

This journal is © The Royal Society of Chemistry 2014

R27	2.05393	-0.00073	0.00000	-0.00146	-0.00146
2.05248					
R28	2.61557	-0.00023	0.00000	0.00270	0.00270
2.61827					
R29	2.05325	-0.00024	0.00000	-0.00033	-0.00033
2.05293					
R30	2.66907	-0.00054	0.00000	-0.00378	-0.00378
2.66528					
R31	2.05325	-0.00012	0.00000	-0.00035	-0.00035
2.05291					
R32	2.61557	-0.00069	0.00000	0.00105	0.00105
2.61662					
R33	2.05393	-0.00019	0.00000	-0.00026	-0.00026
2.05367					
R34	2.68595	0.00005	0.00000	-0.00605	-0.00608
2.67987					
R35	2.66894	-0.00041	0.00000	-0.00318	-0.00318
2.66576					
R36	2.66895	0.00006	0.00000	-0.00288	-0.00288
2.66607					
R37	2.05546	-0.00090	0.00000	-0.00228	-0.00228
2.05318					
R38	2.61902	-0.00034	0.00000	0.00206	0.00206
2.62108					
R39	2.05358	-0.00026	0.00000	-0.00040	-0.00040
2.05318					
R40	2.66823	-0.00056	0.00000	-0.00380	-0.00379
2.66443					
R41	2.05358	-0.00012	0.00000	-0.00032	-0.00032
2.05325					
R42	2.61902	-0.00090	0.00000	0.00056	0.00055
2.61958					
R43	2.05546	-0.00022	0.00000	-0.00038	-0.00038
2.05508					
R44	2.64336	0.00042	0.00000	0.00589	0.00586
2.64922					
R45	2.27474	-0.00467	0.00000	-0.00560	-0.00560
2.26914					
R46	2.64336	-0.00198	0.00000	-0.00964	-0.00966
2.63370					
R47	2.27474	-0.00117	0.00000	-0.00110	-0.00110
2.27364					
R48	2.16676	0.03804	0.00000	0.02575	0.02575
2.19251					
A1	2.03412	-0.00297	0.00000	-0.00689	-0.00691
2.02721					
A2	2.15958	0.00287	0.00000	0.00575	0.00576
2.16534					
A3	2.08631	0.00018	0.00000	0.00136	0.00137
2.08767					
A4	2.07044	0.00173	0.00000	-0.01099	-0.01116
2.05927					

This journal is © The Royal Society of Chemistry 2014

A5	2.05377	-0.00079	0.00000	0.00681	0.00650
2.06027					
A6	2.06014	-0.00261	0.00000	-0.01194	-0.01214
2.04800					
A7	2.03412	0.00223	0.00000	0.00372	0.00367
2.03779					
A8	2.08631	-0.00041	0.00000	0.00175	0.00176
2.08807					
A9	2.15958	-0.00175	0.00000	-0.00530	-0.00526
2.15432					
A10	2.05377	-0.00050	0.00000	-0.00606	-0.00630
2.04747					
A11	2.07044	0.00054	0.00000	-0.00674	-0.00700
2.06343					
A12	2.06014	-0.00014	0.00000	-0.00407	-0.00432
2.05582					
A13	2.18896	-0.00055	0.00000	-0.01125	-0.01145
2.17751					
A14	2.07598	-0.00059	0.00000	-0.00670	-0.00693
2.06905					
A15	1.86833	0.00192	0.00000	0.00036	0.00028
1.86861					
A16	2.18896	-0.00150	0.00000	-0.00394	-0.00395
2.18501					
A17	1.86833	-0.00151	0.00000	-0.00362	-0.00361
1.86472					
A18	2.07598	0.00169	0.00000	0.00011	0.00001
2.07599					
A19	2.08462	0.00059	0.00000	0.00513	0.00513
2.08975					
A20	2.09348	-0.00056	0.00000	-0.00306	-0.00307
2.09041					
A21	2.10506	-0.00002	0.00000	-0.00206	-0.00206
2.10300					
A22	2.09182	-0.00056	0.00000	-0.00379	-0.00379
2.08803					
A23	2.10287	0.00062	0.00000	0.00304	0.00304
2.10591					
A24	2.08841	-0.00005	0.00000	0.00076	0.00076
2.08918					
A25	2.08842	0.00020	0.00000	0.00182	0.00182
2.09024					
A26	2.10287	-0.00022	0.00000	-0.00274	-0.00274
2.10013					
A27	2.09182	0.00003	0.00000	0.00094	0.00094
2.09275					
A28	2.09348	0.00042	0.00000	-0.00029	-0.00030
2.09318					
A29	2.08462	-0.00044	0.00000	-0.00059	-0.00059
2.08403					
A30	2.10506	0.00002	0.00000	0.00088	0.00089
2.10595					

This journal is © The Royal Society of Chemistry 2014

A31	2.03366	0.00180	0.00000	0.00178	0.00171
2.03538					
A32	2.16013	-0.00163	0.00000	-0.00526	-0.00522
2.15491					
A33	2.08585	-0.00012	0.00000	0.00335	0.00338
2.08923					
A34	2.03366	-0.00220	0.00000	-0.00447	-0.00452
2.02915					
A35	2.16013	0.00231	0.00000	0.00539	0.00540
2.16552					
A36	2.08585	-0.00002	0.00000	-0.00012	-0.00014
2.08571					
A37	2.08494	0.00047	0.00000	0.00486	0.00486
2.08980					
A38	2.09635	-0.00053	0.00000	-0.00279	-0.00279
2.09357					
A39	2.10175	0.00006	0.00000	-0.00209	-0.00209
2.09966					
A40	2.09333	-0.00061	0.00000	-0.00425	-0.00425
2.08907					
A41	2.10059	0.00066	0.00000	0.00338	0.00338
2.10398					
A42	2.08926	-0.00006	0.00000	0.00087	0.00087
2.09014					
A43	2.08926	0.00028	0.00000	0.00208	0.00208
2.09134					
A44	2.10059	-0.00033	0.00000	-0.00297	-0.00297
2.09762					
A45	2.09333	0.00006	0.00000	0.00089	0.00090
2.09422					
A46	2.09635	0.00036	0.00000	-0.00080	-0.00081
2.09554					
A47	2.08494	-0.00043	0.00000	-0.00073	-0.00072
2.08422					
A48	2.10175	0.00008	0.00000	0.00153	0.00153
2.10328					
A49	1.88562	-0.00003	0.00000	-0.00131	-0.00130
1.88432					
A50	2.27620	0.00017	0.00000	0.00171	0.00171
2.27791					
A51	2.12132	-0.00013	0.00000	-0.00037	-0.00038
2.12094					
A52	1.88562	-0.00015	0.00000	0.00059	0.00062
1.88624					
A53	2.27621	-0.00077	0.00000	-0.00656	-0.00658
2.26963					
A54	2.12132	0.00093	0.00000	0.00594	0.00592
2.12723					
A55	1.90526	-0.00028	0.00000	0.00279	0.00277
1.90803					
A56	3.14159	0.00192	0.00000	0.01875	0.01875
3.16034					

This journal is © The Royal Society of Chemistry 2014

A57	3.14159	-0.00049	0.00000	-0.01153	-0.01153	3.13006
D1	-0.57102	0.00061	0.00000	-0.01821	-0.01821	-0.58923
D2	3.04203	0.00504	0.00000	0.02090	0.02099	3.06302
D3	2.65673	-0.00045	0.00000	-0.02117	-0.02117	2.63556
D4	-0.01341	0.00398	0.00000	0.01794	0.01803	0.00462
D5	0.00000	0.00016	0.00000	0.00103	0.00108	0.00108
D6	-3.05925	-0.00067	0.00000	-0.00093	-0.00090	-3.06015
D7	3.05925	0.00132	0.00000	0.00411	0.00415	3.06341
D8	0.00000	0.00049	0.00000	0.00216	0.00217	0.00217
D9	-0.06093	0.00047	0.00000	0.00021	0.00021	-0.06072
D10	3.08782	0.00030	0.00000	0.00012	0.00012	3.08794
D11	-3.11394	-0.00048	0.00000	-0.00246	-0.00247	-3.11641
D12	0.03482	-0.00064	0.00000	-0.00255	-0.00256	0.03226
D13	0.57087	-0.00071	0.00000	0.01319	0.01317	0.58404
D14	-2.66181	0.00053	0.00000	0.02332	0.02327	-2.63854
D15	-3.04390	-0.00466	0.00000	-0.02100	-0.02072	-3.06461
D16	0.00661	-0.00342	0.00000	-0.01087	-0.01062	-0.00401
D17	-3.04203	-0.00152	0.00000	-0.01410	-0.01403	-3.05606
D18	0.57102	-0.00126	0.00000	0.02458	0.02455	0.59557
D19	0.01342	-0.00057	0.00000	-0.01166	-0.01159	0.00183
D20	-2.65673	-0.00032	0.00000	0.02702	0.02700	-2.62973
D21	-0.03482	-0.00004	0.00000	-0.00054	-0.00055	-0.03537
D22	3.11394	0.00019	0.00000	0.00053	0.00053	3.11447
D23	-3.08782	-0.00113	0.00000	-0.00313	-0.00314	-3.09096
D24	0.06093	-0.00090	0.00000	-0.00206	-0.00206	0.05887
D25	-0.57087	0.00104	0.00000	-0.02974	-0.02979	-0.60065

This journal is © The Royal Society of Chemistry 2014

D26	2.66181	0.00032	0.00000	-0.02839	-0.02839	2.63342
D27	3.04390	0.00139	0.00000	0.00962	0.00952	3.05342
D28	-0.00661	0.00068	0.00000	0.01097	0.01092	0.00431
D29	0.00000	0.00175	0.00000	-0.01380	-0.01374	-0.01374
D30	2.56664	0.00007	0.00000	-0.02658	-0.02651	2.54013
D31	-2.56664	0.00047	0.00000	0.01808	0.01802	-2.54861
D32	0.00000	-0.00121	0.00000	0.00530	0.00526	0.00526
D33	-2.69646	-0.00033	0.00000	0.02245	0.02245	-2.67401
D34	0.45470	-0.00051	0.00000	0.02662	0.02660	0.48130
D35	-0.08589	0.00079	0.00000	-0.00897	-0.00896	-0.09485
D36	3.06526	0.00061	0.00000	-0.00480	-0.00481	3.06046
D37	0.08589	0.00116	0.00000	-0.00046	-0.00045	0.08544
D38	-3.06526	0.00147	0.00000	0.00351	0.00350	-3.06176
D39	2.69645	-0.00154	0.00000	-0.01372	-0.01370	2.68275
D40	-0.45470	-0.00122	0.00000	-0.00976	-0.00975	-0.46445
D41	3.12047	0.00019	0.00000	0.00000	0.00001	3.12048
D42	-0.03515	0.00030	0.00000	0.00119	0.00119	-0.03396
D43	-0.01387	0.00002	0.00000	-0.00012	-0.00012	-0.01399
D44	3.11369	0.00014	0.00000	0.00107	0.00107	3.11476
D45	-3.12759	-0.00015	0.00000	-0.00059	-0.00059	-3.12818
D46	0.00000	0.00017	0.00000	0.00056	0.00057	0.00057
D47	0.00000	-0.00003	0.00000	0.00056	0.00056	0.00056
D48	3.12759	0.00029	0.00000	0.00171	0.00172	3.12931
D49	0.03515	-0.00029	0.00000	-0.00089	-0.00089	0.03426
D50	-3.11369	-0.00053	0.00000	-0.00198	-0.00199	-3.11568
D51	-3.12047	0.00004	0.00000	0.00027	0.00028	-3.12019

This journal is © The Royal Society of Chemistry 2014

D52	0.01388	-0.00021	0.00000	-0.00082	-0.00082	0.01306
D53	0.00000	0.00030	0.00000	0.00921	0.00922	0.00922
D54	-3.05459	-0.00103	0.00000	-0.00078	-0.00071	-3.05530
D55	3.05459	0.00089	0.00000	0.00745	0.00740	3.06200
D56	0.00000	-0.00043	0.00000	-0.00254	-0.00252	-0.00252
D57	3.07782	0.00085	0.00000	-0.00069	-0.00076	3.07706
D58	-0.08171	0.00069	0.00000	-0.00076	-0.00081	-0.08251
D59	0.02988	0.00002	0.00000	0.00079	0.00078	0.03067
D60	-3.12964	-0.00014	0.00000	0.00072	0.00073	-3.12891
D61	0.08171	-0.00065	0.00000	-0.00622	-0.00622	0.07549
D62	-3.07781	-0.00058	0.00000	-0.00720	-0.00721	-3.08503
D63	3.12964	0.00053	0.00000	0.00400	0.00398	3.13362
D64	-0.02988	0.00060	0.00000	0.00302	0.00299	-0.02690
D65	-3.11398	-0.00016	0.00000	-0.00022	-0.00021	-3.11419
D66	0.03014	-0.00032	0.00000	-0.00161	-0.00160	0.02854
D67	0.00951	-0.00008	0.00000	-0.00113	-0.00114	0.00837
D68	-3.12956	-0.00024	0.00000	-0.00252	-0.00253	-3.13209
D69	3.13907	0.00016	0.00000	0.00070	0.00069	3.13977
D70	0.00000	-0.00012	0.00000	-0.00025	-0.00024	-0.00024
D71	0.00000	0.00000	0.00000	-0.00068	-0.00069	-0.00069
D72	-3.13907	-0.00028	0.00000	-0.00164	-0.00163	-3.14070
D73	-0.03014	0.00025	0.00000	0.00069	0.00068	-0.02946
D74	3.12956	0.00042	0.00000	0.00078	0.00075	3.13031
D75	3.11398	-0.00003	0.00000	-0.00027	-0.00026	3.11371
D76	-0.00951	0.00014	0.00000	-0.00018	-0.00019	-0.00970
D77	-0.14200	-0.00066	0.00000	-0.00577	-0.00578	-0.14778

```
   D78        3.00814  -0.00095   0.00000  -0.00932  -0.00932
2.99882
   D79        0.14200  -0.00013   0.00000   0.00907   0.00907
0.15107
   D80       -3.00814   0.00002   0.00000   0.00527   0.00524  -
3.00289
         Item               Value     Threshold  Converged?
 Maximum Force            0.047833     0.000450     NO
 RMS     Force            0.004721     0.000300     NO
 Maximum Displacement     0.144228     0.001800     NO
 RMS     Displacement     0.037234     0.001200     NO
 Predicted change in Energy=-7.732636D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.561357    1.120358   -0.739337
    2          6             0        0.516744    0.393728   -1.389474
    3          6             0       -0.560065    1.103817    0.680934
    4          6             0        0.505139    0.373429    1.320320
    5          1             0        0.469717    0.285569    2.405459
    6          6             0       -0.007055   -1.635785    0.703904
    7          1             0        0.769038   -2.091387    1.305908
    8          6             0       -0.041273   -1.645864   -0.710294
    9          1             0        0.706388   -2.097067   -1.348826
   10          6             0       -1.627838    1.736315   -1.428702
   11          1             0       -1.642678    1.729520   -2.514703
   12          6             0       -2.643510    2.352340   -0.715533
   13          1             0       -3.453081    2.842876   -1.248591
   14          6             0       -2.644629    2.335419    0.694773
   15          1             0       -3.454826    2.812281    1.239149
   16          6             0       -1.626893    1.701371    1.387213
   17          1             0       -1.634909    1.664304    2.473308
   18          6             0        1.802626    0.362344    0.685802
   19          6             0        1.816500    0.366585   -0.732251
   20          6             0        3.045431    0.250507   -1.415390
   21          1             0        3.059771    0.245845   -2.501783
   22          6             0        4.230380    0.165642   -0.699493
   23          1             0        5.176392    0.102152   -1.230057
   24          6             0        4.217018    0.159733    0.710388
   25          1             0        5.152140    0.091114    1.259384
   26          6             0        3.015042    0.239271    1.396342
   27          1             0        2.997834    0.224593    2.483607
   28          6             0       -1.470261   -1.731218   -1.105492
   29          6             0       -1.412410   -1.722295    1.174262
   30          8             0       -2.246322   -1.655685    0.059567
   31          8             0       -1.850425   -1.818640    2.290708
```

32	8	0	-1.974604	-1.839669	-2.189807
33	6	0	0.500256	0.301179	-2.811743
34	7	0	0.508861	0.219965	-3.969092

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.453607	0.000000			
3	C	1.420368	2.439331	0.000000		
4	C	2.436699	2.709896	1.441159	0.000000	
5	H	3.413169	3.796765	2.168863	1.089265	0.000000
6	C	3.160145	2.962351	2.794954	2.163159	2.610403
7	H	4.033395	3.674851	3.516594	2.478945	2.636005
8	C	2.814838	2.220947	3.124965	2.915391	3.701278
9	H	3.511477	2.498334	3.996184	3.642553	4.452822
10	C	1.411386	2.530477	2.447603	3.736867	4.604909
11	H	2.166162	2.777334	3.431567	4.599946	5.545737
12	C	2.419444	3.778567	2.801727	4.239667	4.868708
13	H	3.404185	4.666657	3.888050	5.325878	5.939717
14	C	2.805899	4.255412	2.421248	3.763210	4.102131
15	H	3.892194	5.341576	3.407359	4.651442	4.811091
16	C	2.448501	3.743675	1.412099	2.512661	2.727104
17	H	3.430667	4.600550	2.163802	2.752371	2.516936
18	C	2.862520	2.441567	2.476311	1.444372	2.177099
19	C	2.494479	1.456724	2.861584	2.435727	3.415495
20	C	3.771287	2.532872	4.257031	3.735278	4.608081
21	H	4.121111	2.779584	4.895816	4.599011	5.548962
22	C	4.886083	3.784070	5.072880	4.242669	4.878287
23	H	5.848017	4.671482	6.128797	5.329035	5.950076
24	C	5.085014	4.261009	4.869567	3.767722	4.114774
25	H	6.139892	5.347421	5.830047	4.655967	4.824560
26	C	4.257707	3.745146	3.747084	2.514635	2.738455
27	H	4.884424	4.602735	4.084275	2.754799	2.530059
28	C	3.015238	2.923051	3.472348	3.770452	4.489735
29	C	3.530839	3.843427	2.992787	2.844360	3.014924
30	O	3.344214	3.732874	3.293086	3.643808	4.080262
31	O	4.413680	4.903244	3.577311	3.360878	3.134314
32	O	3.586488	3.440264	4.348125	4.834038	5.622083
33	C	2.468389	1.425372	3.737285	4.132698	5.217314
34	N	3.519573	2.585476	4.852478	5.291640	6.375009

		6	7	8	9	10
6	C	0.000000				
7	H	1.082729	0.000000			
8	C	1.414648	2.218144	0.000000		
9	H	2.221595	2.655479	1.081806	0.000000	
10	C	4.306507	5.279622	3.804265	4.488853	0.000000
11	H	4.935582	5.917158	4.148928	4.638980	1.086123
12	C	4.987067	5.956376	4.770462	5.605364	1.385528
13	H	5.978773	6.978445	5.663831	6.458658	2.142062
14	C	4.767320	5.623453	4.960070	5.920519	2.429390
15	H	5.653220	6.472360	5.943714	6.936498	3.407788
16	C	3.771922	4.486882	4.256490	5.230510	2.816132

This journal is © The Royal Society of Chemistry 2014

17	H	4.083049	4.609447	4.861297	5.851350	3.902681
18	C	2.695885	2.733793	3.062996	3.374930	4.257583
19	C	3.065515	3.360490	2.738933	2.771660	3.771561
20	C	4.167394	4.251104	3.690680	3.314612	4.903799
21	H	4.818961	5.020818	4.050243	3.515247	5.034549
22	C	4.813576	4.593113	4.639901	4.237925	6.108803
23	H	5.799030	5.537823	5.527181	4.983132	7.000535
24	C	4.589850	4.160618	4.838549	4.653819	6.420565
25	H	5.468824	4.896637	5.819644	5.599608	7.476670
26	C	3.623311	3.238005	4.163257	4.280690	5.637229
27	H	3.956983	3.423195	4.789132	5.032730	6.244062
28	C	2.328946	3.310443	1.485084	2.220553	3.486126
29	C	1.484500	2.216365	2.331825	3.315981	4.334030
30	O	2.330210	3.291747	2.335599	3.301043	3.755414
31	O	2.439138	2.811728	3.508404	4.456571	5.149879
32	O	3.505193	4.450951	2.442190	2.821564	3.672491
33	C	4.045858	4.769870	2.915530	2.816771	2.915682
34	N	5.054391	5.765038	3.795225	3.503348	3.649436

		11	12	13	14	15
11	H	0.000000				
12	C	2.150950	0.000000			
13	H	2.473896	1.086361	0.000000		
14	C	3.416395	1.410408	2.165126	0.000000	
15	H	4.306699	2.165770	2.487928	1.086352	0.000000
16	C	3.902049	2.424626	3.403741	1.384657	2.144151
17	H	4.988443	3.414582	4.306658	2.152467	2.480543
18	C	4.897195	5.068723	6.125143	4.865304	5.826593
19	C	4.123183	4.882130	5.845264	5.080785	6.136345
20	C	5.037294	6.105043	6.998489	6.416886	7.474129
21	H	4.930972	6.336831	7.122661	6.864727	7.938586
22	C	6.342989	7.213340	8.155039	7.342864	8.356160
23	H	7.127296	8.153462	9.054265	8.358278	9.377617
24	C	6.870333	7.342181	8.358664	7.198336	8.134666
25	H	7.943403	8.353777	9.376137	8.132975	9.026905
26	C	6.261906	6.398773	7.457281	6.076011	6.964502
27	H	6.984429	6.825435	7.899304	6.284337	7.062693
28	C	3.740629	4.266619	4.987423	4.599743	5.484453
29	C	5.057322	4.657208	5.556558	4.267707	4.973736
30	O	4.295447	4.101562	4.837830	4.060918	4.776465
31	O	5.977003	5.202263	6.068349	4.520395	5.012514
32	O	3.599283	4.493759	4.999801	5.118701	5.965688
33	C	2.592403	4.299375	4.953033	5.130701	6.193386
34	N	3.003852	5.007007	5.475196	6.014257	7.039652

		16	17	18	19	20
16	C	0.000000				
17	H	1.086757	0.000000			
18	C	3.747876	4.087411	0.000000		
19	C	4.258020	4.885889	1.418127	0.000000	
20	C	5.638280	6.247110	2.443784	1.410824	0.000000
21	H	6.261602	6.985956	3.428510	2.165998	1.086497
22	C	6.404721	6.834784	2.802092	2.422450	1.387017
23	H	7.462726	7.908796	3.888510	3.406847	2.144144

24	C	6.081614	6.294178	2.423003	2.808287	2.428948
25	H	6.968827	7.071957	3.409076	3.894738	3.408525
26	C	4.866763	4.981227	1.410662	2.446144	2.811919
27	H	4.977053	4.851308	2.163238	3.428914	3.899373
28	C	4.245089	4.936040	4.278262	3.917000	4.941127
29	C	3.436981	3.634017	3.862741	4.292327	5.520017
30	O	3.662808	4.149976	4.567120	4.606851	5.814784
31	O	3.640981	3.494379	4.547218	5.230662	6.479655
32	O	5.045289	5.842762	5.233112	4.622176	5.492660
33	C	4.910858	5.860785	3.732657	2.461923	2.903495
34	N	5.953655	6.941642	4.833440	3.494075	3.599516

		21	22	23	24	25
21	H	0.000000				
22	C	2.150583	0.000000			
23	H	2.473463	1.086494	0.000000		
24	C	3.415358	1.409956	2.165419	0.000000	
25	H	4.306776	2.166193	2.489583	1.086535	0.000000
26	C	3.898387	2.423838	3.404145	1.386220	2.146601
27	H	4.985819	3.413908	4.307250	2.152887	2.481446
28	C	5.136107	6.021645	6.895995	6.262448	7.264277
29	C	6.114514	6.238296	7.247183	5.953794	6.810948
30	O	6.191200	6.770603	7.736265	6.744929	7.695979
31	O	7.165200	7.060797	8.090821	6.574590	7.331214
32	O	5.458172	6.689106	7.471850	7.123547	8.149560
33	C	2.578809	4.288799	4.940404	5.122473	6.185323
34	N	2.942925	4.954082	5.413136	5.970895	6.993826

		26	27	28	29	30
26	C	0.000000				
27	H	1.087500	0.000000			
28	C	5.500904	6.055634	0.000000		
29	C	4.847617	4.995499	2.280505	0.000000	
30	O	5.749763	6.075573	1.401906	1.393696	0.000000
31	O	5.357952	5.264753	3.418530	1.203159	2.271844
32	O	6.486835	7.129314	1.200776	3.412741	2.273184
33	C	4.902649	5.855296	3.305278	4.862198	4.429157
34	N	5.921926	6.916092	3.990519	5.823895	5.228690

		31	32	33	34
31	O	0.000000			
32	O	4.482285	0.000000		
33	C	6.004526	3.330911	0.000000	
34	N	6.993371	3.684502	1.160227	0.000000

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

This journal is © The Royal Society of Chemistry 2014

1	6	0	-0.552942	0.679748	1.015783
2	6	0	0.554807	1.133482	0.191168
3	6	0	-0.640085	-0.721482	1.231206
4	6	0	0.374633	-1.537260	0.613312
5	1	0	0.270828	-2.617791	0.703744
6	6	0	-0.121980	-1.224923	-1.468772
7	1	0	0.609777	-1.940895	-1.821221
8	6	0	-0.068388	0.168076	-1.709416
9	1	0	0.712115	0.676100	-2.259899
10	6	0	-1.567182	1.526195	1.512627
11	1	0	-1.514603	2.595347	1.328745
12	6	0	-2.617849	0.988449	2.238310
13	1	0	-3.386887	1.644335	2.636525
14	6	0	-2.706784	-0.402878	2.451734
15	1	0	-3.543546	-0.810062	3.012263
16	6	0	-1.741596	-1.252215	1.937618
17	1	0	-1.817510	-2.327153	2.078276
18	6	0	1.708813	-0.996322	0.496866
19	6	0	1.810809	0.399763	0.269648
20	6	0	3.078349	0.975822	0.041787
21	1	0	3.160101	2.043863	-0.140099
22	6	0	4.215447	0.182194	0.073066
23	1	0	5.191778	0.634467	-0.077585
24	6	0	4.114451	-1.206147	0.297304
25	1	0	5.012783	-1.816999	0.317760
26	6	0	2.873204	-1.792630	0.489533
27	1	0	2.788309	-2.864495	0.652486
28	6	0	-1.470971	0.633657	-1.855933
29	6	0	-1.554765	-1.613286	-1.475235
30	8	0	-2.316968	-0.452151	-1.590130
31	8	0	-2.062403	-2.700572	-1.387452
32	8	0	-1.908222	1.715552	-2.139089
33	6	0	0.625619	2.519886	-0.132184
34	7	0	0.705150	3.645697	-0.401165

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3953093      0.2675534
0.2454824
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1869.1084163424 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Initial guess read from the read-write file:
```

This journal is © The Royal Society of Chemistry 2014

```
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1011.05854662     A.U. after   18 cycles
            Convg  =    0.7489D-08             -V/T =  2.0093
```

```
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.001939611    0.001513515    0.000258124
    2          6          -0.000088682    0.001224946    0.008040885
    3          6           0.000297764   -0.000209814   -0.000065922
    4          6          -0.000103586   -0.001318107    0.000006473
    5          1          -0.000102992   -0.000528772   -0.000577774
    6          6           0.000677018    0.002303938    0.000397826
    7          1           0.000161412    0.000416880   -0.000142059
    8          6          -0.000871354   -0.003633065    0.001104117
    9          1          -0.000025992    0.000014111   -0.000314235
   10          6           0.000047962    0.000102426   -0.000165617
   11          1          -0.000003509    0.000076422    0.000087413
   12          6           0.000071456   -0.000099612    0.000260445
   13          1           0.000059773   -0.000015042   -0.000037610
   14          6          -0.000048028    0.000084939    0.000002239
   15          1           0.000025588   -0.000002488   -0.000000440
   16          6           0.000034954    0.000003696   -0.000068823
   17          1           0.000059789   -0.000040405   -0.000043929
   18          6          -0.000737797   -0.000294522   -0.000020011
   19          6           0.003030191    0.000545725    0.000413344
   20          6           0.000044060    0.000183919   -0.000239311
   21          1          -0.000001364   -0.000017688    0.000133735
   22          6          -0.000125492    0.000015658    0.000202172
   23          1          -0.000066193    0.000012165   -0.000048525
   24          6           0.000016388    0.000009600    0.000060414
   25          1          -0.000023308    0.000011312   -0.000002243
   26          6           0.000123117    0.000024291   -0.000063737
   27          1          -0.000053038    0.000037216   -0.000039364
   28          6          -0.000675924    0.000181390   -0.000696465
   29          6          -0.000751094   -0.000237522   -0.000131025
   30          8           0.000242187    0.000066866    0.000337766
   31          8           0.000236268    0.000128610   -0.000027515
   32          8           0.000219387   -0.000235860    0.000619452
   33          6          -0.000036565    0.000073502   -0.001839043
   34          7           0.000307216   -0.000398231   -0.007400754
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.008040885 RMS     0.001281966


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.008772136 RMS     0.000910189
 Search for a saddle point.
 Step number   2 out of a maximum of 195
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
```

This journal is © The Royal Society of Chemistry 2014

```
 Update second derivatives using D2CorX and points  1  2
     Eigenvalues ---   -0.02476   0.00084   0.00741   0.00768
0.01116
     Eigenvalues ---    0.01218   0.01481   0.01543   0.01605
0.01646
     Eigenvalues ---    0.01743   0.01809   0.01903   0.01919
0.01946
     Eigenvalues ---    0.02013   0.02104   0.02166   0.02222
0.02276
     Eigenvalues ---    0.02399   0.02475   0.02493   0.02514
0.02714
     Eigenvalues ---    0.02759   0.02770   0.02778   0.03432
0.03999
     Eigenvalues ---    0.05469   0.06598   0.06991   0.07526
0.08527
     Eigenvalues ---    0.10398   0.11115   0.11161   0.11193
0.11823
     Eigenvalues ---    0.11898   0.12501   0.12521   0.12652
0.12705
     Eigenvalues ---    0.12928   0.14247   0.16413   0.17476
0.18080
     Eigenvalues ---    0.19151   0.19178   0.19205   0.19398
0.19570
     Eigenvalues ---    0.19764   0.20342   0.20990   0.23535
0.23972
     Eigenvalues ---    0.25132   0.25205   0.26187   0.27958
0.28543
     Eigenvalues ---    0.29532   0.30087   0.31009   0.31798
0.33466
     Eigenvalues ---    0.34200   0.35307   0.35875   0.35904
0.36040
     Eigenvalues ---    0.36126   0.36226   0.36265   0.36292
0.36350
     Eigenvalues ---    0.37234   0.38035   0.39103   0.40157
0.40800
     Eigenvalues ---    0.41731   0.42419   0.42902   0.44745
0.47343
     Eigenvalues ---    0.47622   0.50294   0.50637   0.88539
0.89746
     Eigenvalues ---
1.375101000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
          1             -0.05136   0.02363   0.14250   0.01820
0.38329
                           R6        R7        R8        R9        R10
          1              0.13277  -0.05364  -0.03644  -0.05477
0.17581
                           R11       R12       R13       R14       R15
          1              0.01902  -0.00727   0.43832   0.18106  -
0.05465
                           R16       R17       R18       R19       R20
          1              0.31507  -0.00694  -0.09329   0.18551  -
0.01081
                           R21       R22       R23       R24       R25
          1             -0.00812  -0.00837   0.13052  -0.00868  -
0.07495
                           R26       R27       R28       R29       R30
          1              0.05408  -0.00027  -0.01429   0.00002
0.01582
                           R31       R32       R33       R34       R35
          1             -0.00010  -0.01539  -0.00018   0.02032
0.01825
                           R36       R37       R38       R39       R40
          1              0.01786   0.00002  -0.01381   0.00007
0.01525
                           R41       R42       R43       R44       R45
          1             -0.00006  -0.01487  -0.00007  -0.00010
0.00213
```

This journal is © The Royal Society of Chemistry 2014

	R46	R47	R48	A1	A2
1	0.00101	0.00210	-0.00099	0.02223	-0.01173
	A3	A4	A5	A6	A7
1	-0.00966	0.04682	0.02068	0.02155	0.01899
	A8	A9	A10	A11	A12
1	-0.00469	-0.01341	0.02484	0.05375	0.02190
	A13	A14	A15	A16	A17
1	0.05549	0.03235	0.01679	0.04644	0.01273
	A18	A19	A20	A21	A22
1	0.02835	-0.00634	0.00623	0.00011	0.00084
	A23	A24	A25	A26	A27
1	0.00262	-0.00346	-0.00238	0.00093	0.00147
	A28	A29	A30	A31	A32
1	0.00466	-0.00587	0.00120	0.01940	-0.01432
	A33	A34	A35	A36	A37
1	-0.00424	0.02349	-0.01342	-0.00944	-0.00639
	A38	A39	A40	A41	A42
1	0.00639	-0.00004	0.00124	0.00209	-0.00332
	A43	A44	A45	A46	A47
1	-0.00225	0.00044	0.00182	0.00480	-0.00577
	A48	A49	A50	A51	A52
1	0.00093	-0.00371	0.00301	0.00070	-0.00482
	A53	A54	A55	A56	A57
1	0.00415	0.00077	-0.01346	-0.00489	0.01665
	D1	D2	D3	D4	D5
1	0.16171	-0.02614	0.15026	-0.03759	0.00220
	D6	D7	D8	D9	D10
1	-0.00907	0.01292	0.00165	0.01047	0.01066
	D11	D12	D13	D14	D15
1	-0.00277	-0.00258	-0.16066	-0.15191	0.02554
	D16	D17	D18	D19	D20
1	0.03429	0.04470	-0.16466	0.05696	-0.15240
	D21	D22	D23	D24	D25
1	0.00047	0.00255	-0.01318	-0.01111	0.16514
	D26	D27	D28	D29	D30

```
          1              0.15465  -0.04615  -0.05664   0.01350
0.16718
                           D31       D32       D33       D34       D35
          1             -0.16320  -0.00951  -0.13998  -0.14866
0.03368
                           D36       D37       D38       D39       D40
          1              0.02499  -0.01746  -0.01860   0.13249
0.13135
                           D41       D42       D43       D44       D45
          1              0.00088   0.00117   0.00110   0.00139  -
0.00075
                           D46       D47       D48       D49       D50
          1              0.00078  -0.00043   0.00110  -0.00156  -
0.00369
                           D51       D52       D53       D54       D55
          1             -0.00006  -0.00219  -0.00361  -0.01165
0.00584
                           D56       D57       D58       D59       D60
          1             -0.00220   0.01246   0.00952   0.00050  -
0.00244
                           D61       D62       D63       D64       D65
          1             -0.00633  -0.00799   0.00411   0.00245
0.00046
                           D66       D67       D68       D69       D70
          1             -0.00081  -0.00128  -0.00255   0.00113  -
0.00077
                           D71       D72       D73       D74       D75
          1             -0.00014  -0.00204   0.00090   0.00394  -
0.00100
                           D76       D77       D78       D79       D80
          1              0.00204   0.04159   0.04259  -0.04777  -
0.03991
 RFO step:  Lambda0=1.216146210D-05 Lambda=-1.84885780D-03.
 Linear search not attempted -- option 19 set.
 Maximum step size (   0.300) exceeded in Quadratic search.
    -- Step size scaled by   0.422
 Iteration  1 RMS(Cart)=  0.02029179 RMS(Int)=  0.00022291
 Iteration  2 RMS(Cart)=  0.00028138 RMS(Int)=  0.00011866
 Iteration  3 RMS(Cart)=  0.00000008 RMS(Int)=  0.00011866
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.74692   0.00135   0.00000  -0.00600  -0.00598
2.74094
    R2        2.68411   0.00007   0.00000   0.00155   0.00158
2.68568
    R3        5.31927   0.00066   0.00000   0.06978   0.06977
5.38905
    R4        2.66713  -0.00009   0.00000   0.00210   0.00210
2.66924
    R5        4.19698   0.00104   0.00000   0.13781   0.13768
4.33466
```

This journal is © The Royal Society of Chemistry 2014

R6	4.72117	-0.00121	0.00000	0.07879	0.07877
4.79994					
R7	2.75281	0.00111	0.00000	-0.00481	-0.00480
2.74801					
R8	2.69356	0.00877	0.00000	0.01334	0.01332
2.70688					
R9	2.72340	0.00015	0.00000	0.00148	0.00144
2.72484					
R10	5.28170	0.00014	0.00000	-0.03842	-0.03835
5.24335					
R11	2.66848	-0.00011	0.00000	-0.00040	-0.00040
2.66808					
R12	2.05841	-0.00002	0.00000	-0.00136	-0.00130
2.05712					
R13	4.08778	-0.00061	0.00000	-0.08400	-0.08395
4.00383					
R14	4.68453	-0.00005	0.00000	-0.07266	-0.07264
4.61188					
R15	2.72947	0.00001	0.00000	0.00048	0.00043
2.72990					
R16	4.93295	-0.00088	0.00000	-0.10634	-0.10646
4.82649					
R17	2.04606	0.00014	0.00000	0.00017	0.00019
2.04625					
R18	2.67330	-0.00010	0.00000	-0.00674	-0.00666
2.66664					
R19	5.09448	-0.00032	0.00000	-0.03576	-0.03559
5.05889					
R20	2.80530	0.00020	0.00000	0.00902	0.00899
2.81429					
R21	5.16612	-0.00109	0.00000	-0.03268	-0.03279
5.13333					
R22	2.04432	0.00043	0.00000	-0.00153	-0.00154
2.04278					
R23	5.17583	0.00183	0.00000	0.07692	0.07686
5.25269					
R24	2.80640	0.00056	0.00000	-0.00940	-0.00931
2.79709					
R25	5.23768	0.00084	0.00000	0.03722	0.03730
5.27498					
R26	5.32293	0.00100	0.00000	0.07655	0.07659
5.39952					
R27	2.05248	-0.00008	0.00000	-0.00010	-0.00010
2.05237					
R28	2.61827	-0.00002	0.00000	-0.00145	-0.00145
2.61682					
R29	2.05293	-0.00003	0.00000	-0.00002	-0.00002
2.05291					
R30	2.66528	-0.00007	0.00000	0.00100	0.00100
2.66628					
R31	2.05291	-0.00002	0.00000	-0.00005	-0.00005
2.05286					

This journal is © The Royal Society of Chemistry 2014

R32	2.61662	-0.00003	0.00000	-0.00031	-0.00032
2.61631					
R33	2.05367	-0.00005	0.00000	-0.00013	-0.00013
2.05355					
R34	2.67987	-0.00027	0.00000	0.00091	0.00093
2.68080					
R35	2.66576	-0.00003	0.00000	-0.00026	-0.00025
2.66551					
R36	2.66607	-0.00006	0.00000	0.00207	0.00207
2.66814					
R37	2.05318	-0.00014	0.00000	-0.00027	-0.00027
2.05292					
R38	2.62108	-0.00002	0.00000	-0.00148	-0.00149
2.61960					
R39	2.05318	-0.00004	0.00000	-0.00004	-0.00004
2.05313					
R40	2.66443	-0.00005	0.00000	0.00094	0.00093
2.66536					
R41	2.05325	-0.00002	0.00000	-0.00003	-0.00003
2.05323					
R42	2.61958	-0.00015	0.00000	-0.00030	-0.00030
2.61928					
R43	2.05508	-0.00004	0.00000	-0.00002	-0.00002
2.05505					
R44	2.64922	0.00010	0.00000	0.00795	0.00789
2.65711					
R45	2.26914	-0.00063	0.00000	-0.00004	-0.00004
2.26910					
R46	2.63370	-0.00046	0.00000	-0.00837	-0.00849
2.62521					
R47	2.27364	-0.00012	0.00000	-0.00011	-0.00011
2.27353					
R48	2.19251	0.00741	0.00000	0.00294	0.00294
2.19545					
A1	2.02721	-0.00080	0.00000	-0.00011	-0.00011
2.02710					
A2	2.16534	0.00060	0.00000	0.00068	0.00065
2.16599					
A3	2.08767	0.00021	0.00000	0.00016	0.00015
2.08782					
A4	2.05927	0.00030	0.00000	0.00950	0.00928
2.06855					
A5	2.06027	0.00087	0.00000	0.00706	0.00674
2.06701					
A6	2.04800	-0.00103	0.00000	0.00388	0.00348
2.05148					
A7	2.03779	0.00051	0.00000	-0.00038	-0.00039
2.03741					
A8	2.08807	-0.00017	0.00000	-0.00049	-0.00049
2.08758					
A9	2.15432	-0.00033	0.00000	0.00030	0.00028
2.15460					

This journal is © The Royal Society of Chemistry 2014

A10	2.04747	-0.00010	0.00000	-0.00210	-0.00211
2.04535					
A11	2.06343	0.00010	0.00000	-0.00330	-0.00344
2.05999					
A12	2.05582	-0.00009	0.00000	-0.00194	-0.00194
2.05388					
A13	2.17751	-0.00002	0.00000	-0.00539	-0.00561
2.17190					
A14	2.06905	-0.00036	0.00000	-0.00447	-0.00469
2.06435					
A15	1.86861	0.00027	0.00000	-0.00597	-0.00590
1.86271					
A16	2.18501	0.00049	0.00000	0.01944	0.01870
2.20371					
A17	1.86472	-0.00041	0.00000	0.00799	0.00759
1.87231					
A18	2.07599	-0.00001	0.00000	0.00838	0.00740
2.08339					
A19	2.08975	0.00014	0.00000	-0.00007	-0.00008
2.08967					
A20	2.09041	-0.00019	0.00000	-0.00065	-0.00064
2.08977					
A21	2.10300	0.00005	0.00000	0.00071	0.00070
2.10370					
A22	2.08803	-0.00012	0.00000	-0.00038	-0.00038
2.08765					
A23	2.10591	0.00011	0.00000	0.00050	0.00050
2.10641					
A24	2.08918	0.00001	0.00000	-0.00010	-0.00010
2.08907					
A25	2.09024	0.00003	0.00000	-0.00016	-0.00016
2.09008					
A26	2.10013	-0.00004	0.00000	0.00017	0.00017
2.10030					
A27	2.09275	0.00002	0.00000	-0.00002	-0.00002
2.09273					
A28	2.09318	0.00009	0.00000	0.00030	0.00030
2.09348					
A29	2.08403	-0.00012	0.00000	-0.00042	-0.00042
2.08361					
A30	2.10595	0.00003	0.00000	0.00013	0.00012
2.10607					
A31	2.03538	0.00018	0.00000	-0.00023	-0.00020
2.03517					
A32	2.15491	-0.00022	0.00000	0.00028	0.00025
2.15516					
A33	2.08923	0.00002	0.00000	-0.00045	-0.00046
2.08877					
A34	2.02915	-0.00027	0.00000	-0.00011	-0.00010
2.02904					
A35	2.16552	0.00024	0.00000	0.00053	0.00048
2.16601					

A36	2.08571	0.00005	0.00000	0.00029	0.00028	2.08599
A37	2.08980	0.00006	0.00000	-0.00013	-0.00014	2.08966
A38	2.09357	-0.00011	0.00000	-0.00064	-0.00063	2.09293
A39	2.09966	0.00005	0.00000	0.00076	0.00076	2.10042
A40	2.08907	-0.00012	0.00000	-0.00037	-0.00037	2.08870
A41	2.10398	0.00010	0.00000	0.00037	0.00037	2.10435
A42	2.09014	0.00002	0.00000	0.00000	0.00000	2.09014
A43	2.09134	0.00007	0.00000	-0.00017	-0.00017	2.09117
A44	2.09762	-0.00010	0.00000	0.00024	0.00024	2.09786
A45	2.09422	0.00004	0.00000	-0.00007	-0.00007	2.09416
A46	2.09554	0.00004	0.00000	0.00018	0.00018	2.09572
A47	2.08422	-0.00008	0.00000	-0.00026	-0.00026	2.08396
A48	2.10328	0.00004	0.00000	0.00007	0.00006	2.10335
A49	1.88432	0.00011	0.00000	-0.00222	-0.00209	1.88223
A50	2.27791	0.00001	0.00000	0.00509	0.00502	2.28293
A51	2.12094	-0.00012	0.00000	-0.00284	-0.00292	2.11802
A52	1.88624	0.00000	0.00000	0.00126	0.00120	1.88744
A53	2.26963	-0.00024	0.00000	-0.00594	-0.00592	2.26371
A54	2.12723	0.00024	0.00000	0.00462	0.00464	2.13188
A55	1.90803	0.00003	0.00000	-0.00056	-0.00068	1.90736
A56	3.16034	0.00033	0.00000	0.00228	0.00228	3.16262
A57	3.13006	-0.00026	0.00000	-0.00102	-0.00102	3.12905
D1	-0.58923	0.00006	0.00000	0.02209	0.02216	-0.56707
D2	3.06302	0.00008	0.00000	-0.02070	-0.02079	3.04222
D3	2.63556	0.00000	0.00000	0.01177	0.01184	2.64740
D4	0.00462	0.00001	0.00000	-0.03102	-0.03111	-0.02649

This journal is © The Royal Society of Chemistry 2014

D5	0.00108	0.00007	0.00000	-0.01998	-0.01996	-0.01888
D6	-3.06015	-0.00003	0.00000	-0.01234	-0.01234	-3.07249
D7	3.06341	0.00016	0.00000	-0.01011	-0.01010	3.05330
D8	0.00217	0.00005	0.00000	-0.00247	-0.00248	-0.00031
D9	-0.06072	-0.00003	0.00000	0.00964	0.00964	-0.05108
D10	3.08794	-0.00003	0.00000	0.01208	0.01208	3.10002
D11	-3.11641	-0.00006	0.00000	-0.00101	-0.00101	-3.11741
D12	0.03226	-0.00006	0.00000	0.00143	0.00144	0.03369
D13	0.58404	-0.00023	0.00000	-0.01961	-0.01968	0.56436
D14	-2.63854	0.00002	0.00000	-0.00939	-0.00946	-2.64800
D15	-3.06461	0.00030	0.00000	0.02380	0.02383	-3.04079
D16	-0.00401	0.00056	0.00000	0.03402	0.03405	0.03004
D17	-3.05606	-0.00015	0.00000	-0.00236	-0.00241	-3.05848
D18	0.59557	0.00005	0.00000	0.01304	0.01302	0.60859
D19	0.00183	-0.00003	0.00000	-0.01036	-0.01040	-0.00857
D20	-2.62973	0.00016	0.00000	0.00504	0.00504	-2.62469
D21	-0.03537	-0.00002	0.00000	0.00112	0.00113	-0.03423
D22	3.11447	0.00003	0.00000	0.00002	0.00003	3.11449
D23	-3.09096	-0.00017	0.00000	0.00933	0.00932	-3.08164
D24	0.05887	-0.00012	0.00000	0.00823	0.00822	0.06709
D25	-0.60065	-0.00029	0.00000	-0.01057	-0.01056	-0.61121
D26	2.63342	-0.00010	0.00000	-0.00548	-0.00549	2.62793
D27	3.05342	-0.00009	0.00000	0.00496	0.00501	3.05843
D28	0.00431	0.00010	0.00000	0.01004	0.01007	0.01439
D29	-0.01374	-0.00036	0.00000	-0.06362	-0.06391	-0.07765
D30	2.54013	-0.00031	0.00000	-0.00174	-0.00157	2.53856

This journal is © The Royal Society of Chemistry 2014

D31	-2.54861	-0.00007	0.00000	-0.03665	-0.03703	-2.58564
D32	0.00526	-0.00001	0.00000	0.02523	0.02531	0.03057
D33	-2.67401	0.00015	0.00000	0.00607	0.00601	-2.66800
D34	0.48130	0.00017	0.00000	0.01160	0.01155	0.49285
D35	-0.09485	0.00000	0.00000	-0.01925	-0.01925	-0.11410
D36	3.06046	0.00002	0.00000	-0.01372	-0.01371	3.04675
D37	0.08544	0.00000	0.00000	-0.02370	-0.02381	0.06163
D38	-3.06176	0.00008	0.00000	-0.01757	-0.01762	-3.07938
D39	2.68275	0.00027	0.00000	0.03801	0.03793	2.72068
D40	-0.46445	0.00035	0.00000	0.04413	0.04412	-0.42033
D41	3.12048	0.00000	0.00000	-0.00080	-0.00081	3.11967
D42	-0.03396	0.00002	0.00000	0.00095	0.00095	-0.03301
D43	-0.01399	0.00000	0.00000	0.00166	0.00166	-0.01233
D44	3.11476	0.00002	0.00000	0.00341	0.00341	3.11817
D45	-3.12818	-0.00002	0.00000	-0.00155	-0.00155	-3.12974
D46	0.00057	0.00001	0.00000	-0.00231	-0.00231	-0.00174
D47	0.00056	0.00000	0.00000	0.00020	0.00020	0.00076
D48	3.12931	0.00003	0.00000	-0.00056	-0.00056	3.12875
D49	0.03426	-0.00001	0.00000	0.00127	0.00127	0.03553
D50	-3.11568	-0.00006	0.00000	0.00239	0.00238	-3.11329
D51	-3.12019	0.00002	0.00000	0.00051	0.00051	-3.11969
D52	0.01306	-0.00003	0.00000	0.00162	0.00162	0.01468
D53	0.00922	0.00045	0.00000	0.01552	0.01550	0.02472
D54	-3.05530	0.00020	0.00000	0.00578	0.00576	-3.04954
D55	3.06200	0.00025	0.00000	0.01068	0.01068	3.07267
D56	-0.00252	0.00001	0.00000	0.00094	0.00094	-0.00158

This journal is © The Royal Society of Chemistry 2014

```
   D57        3.07706  -0.00018   0.00000  -0.00533  -0.00531
3.07175
   D58       -0.08251  -0.00016   0.00000  -0.00610  -0.00609  -
0.08860
   D59        0.03067   0.00001   0.00000  -0.00011  -0.00011
0.03055
   D60       -3.12891   0.00003   0.00000  -0.00088  -0.00088  -
3.12979
   D61        0.07549  -0.00019   0.00000  -0.01052  -0.01053
0.06496
   D62       -3.08503  -0.00025   0.00000  -0.01131  -0.01131  -
3.09634
   D63        3.13362   0.00005   0.00000  -0.00001  -0.00001
3.13362
   D64       -0.02690   0.00000   0.00000  -0.00079  -0.00079  -
0.02769
   D65       -3.11419   0.00002   0.00000   0.00055   0.00055  -
3.11364
   D66        0.02854  -0.00001   0.00000  -0.00018  -0.00018
0.02836
   D67        0.00837  -0.00004   0.00000  -0.00025  -0.00025
0.00812
   D68       -3.13209  -0.00007   0.00000  -0.00097  -0.00098  -
3.13306
   D69        3.13977   0.00001   0.00000   0.00126   0.00126
3.14103
   D70       -0.00024   0.00003   0.00000   0.00100   0.00100
0.00076
   D71       -0.00069  -0.00002   0.00000   0.00053   0.00054  -
0.00015
   D72       -3.14070  -0.00001   0.00000   0.00028   0.00028  -
3.14042
   D73       -0.02946  -0.00003   0.00000  -0.00088  -0.00087  -
0.03033
   D74        3.13031  -0.00004   0.00000  -0.00010  -0.00009
3.13022
   D75        3.11371  -0.00001   0.00000  -0.00113  -0.00113
3.11258
   D76       -0.00970  -0.00003   0.00000  -0.00035  -0.00035  -
0.01005
   D77       -0.14778  -0.00002   0.00000   0.01181   0.01177  -
0.13601
   D78        2.99882  -0.00009   0.00000   0.00631   0.00625
3.00507
   D79        0.15107   0.00000   0.00000   0.00412   0.00414
0.15521
   D80       -3.00289  -0.00002   0.00000  -0.00096  -0.00099  -
3.00389
         Item               Value     Threshold  Converged?
 Maximum Force            0.008772     0.000450     NO
 RMS     Force            0.000910     0.000300     NO
 Maximum Displacement     0.069925     0.001800     NO
```

This journal is © The Royal Society of Chemistry 2014

```
 RMS     Displacement     0.020366     0.001200     NO
 Predicted change in Energy=-6.945709D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.558305    1.129241   -0.750888
    2          6             0        0.528410    0.425290   -1.404557
    3          6             0       -0.560489    1.096818    0.669942
    4          6             0        0.498745    0.351226    1.303389
    5          1             0        0.459809    0.254532    2.386966
    6          6             0       -0.005646   -1.621388    0.717372
    7          1             0        0.769363   -2.074147    1.323086
    8          6             0       -0.051429   -1.676493   -0.691932
    9          1             0        0.698668   -2.108186   -1.339648
   10          6             0       -1.625658    1.750144   -1.436739
   11          1             0       -1.637089    1.756135   -2.522732
   12          6             0       -2.643185    2.356136   -0.719120
   13          1             0       -3.452528    2.850874   -1.248611
   14          6             0       -2.646296    2.325976    0.691489
   15          1             0       -3.457896    2.796783    1.238988
   16          6             0       -1.629489    1.686031    1.379519
   17          1             0       -1.640208    1.636893    2.465044
   18          6             0        1.800141    0.354478    0.676308
   19          6             0        1.821946    0.376352   -0.741975
   20          6             0        3.055362    0.267781   -1.420515
   21          1             0        3.075310    0.276656   -2.506653
   22          6             0        4.235392    0.174142   -0.699131
   23          1             0        5.184304    0.117060   -1.225178
   24          6             0        4.214284    0.151881    0.710984
   25          1             0        5.146517    0.077655    1.264120
   26          6             0        3.008810    0.222785    1.391405
   27          1             0        2.985824    0.195405    2.478305
   28          6             0       -1.477155   -1.749416   -1.082895
   29          6             0       -1.413621   -1.704423    1.195493
   30          8             0       -2.250325   -1.654170    0.087664
   31          8             0       -1.840938   -1.781637    2.317494
   32          8             0       -1.989701   -1.867696   -2.162302
   33          6             0        0.511573    0.320585   -2.833047
   34          7             0        0.522638    0.229344   -3.991187
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  C    1.450442   0.000000
    3  C    1.421201   2.437252   0.000000
    4  C    2.437769   2.709121   1.441922   0.000000
```

This journal is © The Royal Society of Chemistry 2014

5	H	3.412888	3.795987	2.167632	1.088580	0.000000
6	C	3.166572	2.996113	2.774661	2.118734	2.554069
7	H	4.040516	3.707463	3.500018	2.440504	2.578840
8	C	2.851761	2.293804	3.131309	2.897523	3.670128
9	H	3.522436	2.540020	3.986976	3.615843	4.418953
10	C	1.412499	2.529088	2.449392	3.738764	4.605078
11	H	2.167072	2.776842	3.433210	4.601603	5.545893
12	C	2.419298	3.775845	2.802320	4.240510	4.867554
13	H	3.404155	4.664295	3.888630	5.326678	5.938416
14	C	2.805768	4.252620	2.421133	3.763687	4.100415
15	H	3.892034	5.338816	3.407149	4.651870	4.809293
16	C	2.448690	3.741267	1.411889	2.513340	2.725675
17	H	3.430809	4.598337	2.163300	2.752726	2.515370
18	C	2.863462	2.439736	2.474608	1.444602	2.175507
19	C	2.496501	1.454182	2.861569	2.436187	3.414752
20	C	3.774798	2.531906	4.258132	3.736697	4.608035
21	H	4.124654	2.779101	4.897188	4.600072	5.548770
22	C	4.888193	3.781853	5.072097	4.243110	4.877037
23	H	5.850387	4.669532	6.128136	5.329442	5.948726
24	C	5.086247	4.258630	4.867550	3.767746	4.112850
25	H	6.140936	5.345054	5.827663	4.655983	4.822583
26	C	4.258567	3.743100	3.744909	2.514890	2.736706
27	H	4.884730	4.600907	4.081550	2.755044	2.528357
28	C	3.039931	2.975752	3.466087	3.743157	4.450570
29	C	3.542543	3.881678	2.975061	2.809711	2.960887
30	O	3.363551	3.777862	3.280630	3.613445	4.034199
31	O	4.419652	4.933356	3.555205	3.324399	3.073149
32	O	3.608686	3.488961	4.341958	4.809053	5.585678
33	C	2.476681	1.432421	3.744700	4.136569	5.220688
34	N	3.532392	2.594048	4.863311	5.296033	6.378513

		6	7	8	9	10
6	C	0.000000				
7	H	1.082829	0.000000			
8	C	1.411124	2.211815	0.000000		
9	H	2.228085	2.663889	1.080990	0.000000	
10	C	4.316463	5.289420	3.843797	4.505400	0.000000
11	H	4.956565	5.937372	4.201081	4.667807	1.086070
12	C	4.984056	5.953444	4.793749	5.610990	1.384762
13	H	5.978897	6.978096	5.689852	6.467843	2.141134
14	C	4.749250	5.605954	4.966583	5.914059	2.429535
15	H	5.631194	6.450019	5.944970	6.927128	3.407648
16	C	3.743571	4.460562	4.252969	5.216346	2.816990
17	H	4.042591	4.569674	4.844507	5.828519	3.903454
18	C	2.677050	2.716440	3.070054	3.367794	4.260158
19	C	3.075833	3.373033	2.779606	2.791397	3.775708
20	C	4.184410	4.270570	3.736734	3.347501	4.910153
21	H	4.846566	5.050799	4.109075	3.563398	5.041327
22	C	4.818383	4.599731	4.669232	4.257664	6.113898
23	H	5.807864	5.548580	5.560043	5.008568	7.006233
24	C	4.577372	4.146969	4.848446	4.655378	6.424335
25	H	5.452565	4.877828	5.824244	5.598292	7.480255
26	C	3.597533	3.208690	4.160843	4.269524	5.639993

This journal is © The Royal Society of Chemistry 2014

27	H	3.917973	3.376107	4.772767	5.011424	6.245841
28	C	2.328667	3.307724	1.480157	2.220100	3.520536
29	C	1.489257	2.217745	2.327814	3.324414	4.348291
30	O	2.331564	3.289553	2.333112	3.307553	3.781979
31	O	2.440156	2.808572	3.502862	4.464405	5.158884
32	O	3.505662	4.450055	2.440379	2.821688	3.707794
33	C	4.079736	4.803607	2.981554	2.857302	2.925930
34	N	5.086731	5.797279	3.853161	3.539166	3.667862
		11	12	13	14	15
11	H	0.000000				
12	C	2.150638	0.000000			
13	H	2.473390	1.086353	0.000000		
14	C	3.416787	1.410936	2.165529	0.000000	
15	H	4.306835	2.166129	2.488193	1.086328	0.000000
16	C	3.902888	2.425058	3.404027	1.384490	2.143966
17	H	4.989202	3.414993	4.306912	2.152335	2.480433
18	C	4.900311	5.069221	6.125997	4.863933	5.824811
19	C	4.127931	4.884410	5.848078	5.081441	6.136728
20	C	5.044717	6.109551	7.003895	6.419161	7.476051
21	H	4.939212	6.341978	7.128950	6.867649	7.941262
22	C	6.349351	7.216392	8.159101	7.343150	8.355910
23	H	7.134537	8.157153	9.059203	8.358901	9.377668
24	C	6.875253	7.343624	8.360896	7.196848	8.132443
25	H	7.948261	8.354890	9.378067	8.130854	9.023869
26	C	6.265461	6.399262	7.458245	6.074004	6.961823
27	H	6.986956	6.824809	7.898973	6.281147	7.058654
28	C	3.793099	4.283400	5.009214	4.596101	5.475619
29	C	5.084348	4.654644	5.557114	4.244717	4.943865
30	O	4.338249	4.109476	4.850396	4.045116	4.753394
31	O	5.998764	5.194784	6.064196	4.490542	4.973897
32	O	3.658743	4.511161	5.023903	5.114893	5.956655
33	C	2.602661	4.308671	4.962549	5.139658	6.202395
34	N	3.025206	5.025147	5.495096	6.030379	7.056283
		16	17	18	19	20
16	C	0.000000				
17	H	1.086690	0.000000			
18	C	3.745651	4.084136	0.000000		
19	C	4.257745	4.884716	1.418619	0.000000	
20	C	5.639100	6.246632	2.445355	1.411920	0.000000
21	H	6.262890	6.985995	3.429774	2.166783	1.086357
22	C	6.403391	6.831861	2.802642	2.422281	1.386231
23	H	7.461494	7.905795	3.889033	3.406783	2.143191
24	C	6.078670	6.289440	2.422877	2.807981	2.428955
25	H	6.965231	7.066334	3.408869	3.894408	3.408276
26	C	4.863645	4.976522	1.410527	2.446128	2.812666
27	H	4.972967	4.845434	2.162947	3.428929	3.900112
28	C	4.229537	4.907295	4.273386	3.939439	4.972602
29	C	3.402299	3.581549	3.851868	4.307238	5.541199
30	O	3.634731	4.105518	4.559325	4.625441	5.841131
31	O	3.598503	3.427595	4.529231	5.237746	6.492039
32	O	5.030231	5.815207	5.230552	4.645614	5.528396
33	C	4.918770	5.867929	3.738600	2.468354	2.910137

34	N	5.966412	6.952843	4.840784	3.502455	3.608950
		21	22	23	24	25
21	H	0.000000				
22	C	2.150218	0.000000			
23	H	2.472955	1.086470	0.000000		
24	C	3.415555	1.410449	2.165843	0.000000	
25	H	4.306766	2.166521	2.489897	1.086521	0.000000
26	C	3.898997	2.424296	3.404476	1.386062	2.146405
27	H	4.986422	3.414377	4.307579	2.152773	2.481271
28	C	5.182373	6.039912	6.919466	6.263019	7.260833
29	C	6.146629	6.247395	7.260169	5.945916	6.798229
30	O	6.230646	6.784268	7.754645	6.741032	7.687427
31	O	7.188772	7.060232	8.093800	6.556300	7.306920
32	O	5.511004	6.712806	7.502254	7.129088	8.151710
33	C	2.584804	4.294400	4.945815	5.128225	6.191002
34	N	2.953340	4.962381	5.421674	5.978684	7.001538
		26	27	28	29	30
26	C	0.000000				
27	H	1.087487	0.000000			
28	C	5.489592	6.031803	0.000000		
29	C	4.828085	4.960853	2.279718	0.000000	
30	O	5.734213	6.045936	1.406083	1.389203	0.000000
31	O	5.328733	5.218446	3.419944	1.203099	2.270680
32	O	6.479511	7.109674	1.200756	3.410765	2.275053
33	C	4.908335	5.860720	3.361989	4.902669	4.478648
34	N	5.929030	6.922627	4.046335	5.864316	5.279581
		31	32	33	34	
31	O	0.000000				
32	O	4.483091	0.000000			
33	C	6.040009	3.390404	0.000000		
34	N	7.030646	3.748899	1.161782	0.000000	

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.542922	0.726740	1.001416
2	6	0	0.576945	1.154874	0.185095
3	6	0	-0.644986	-0.670337	1.241356
4	6	0	0.356813	-1.508323	0.630360
5	1	0	0.240795	-2.584855	0.742720
6	6	0	-0.132808	-1.274896	-1.417765
7	1	0	0.591517	-2.009587	-1.746552
8	6	0	-0.080616	0.097623	-1.741397
9	1	0	0.706872	0.595885	-2.289244
10	6	0	-1.550891	1.592825	1.480005

```
   11          1             0       -1.486209    2.658013    1.278171
   12          6             0       -2.607589    1.078459    2.212386
   13          1             0       -3.370909    1.748982    2.596967
   14          6             0       -2.709831   -0.308115    2.452593
   15          1             0       -3.551107   -0.696411    3.019681
   16          6             0       -1.752696   -1.176358    1.955746
   17          1             0       -1.840041   -2.247739    2.115148
   18          6             0        1.698822   -0.986633    0.513202
   19          6             0        1.820131    0.404538    0.263389
   20          6             0        3.096373    0.960129    0.026652
   21          1             0        3.192405    2.023769   -0.172389
   22          6             0        4.221604    0.151796    0.072354
   23          1             0        5.204115    0.588213   -0.084588
   24          6             0        4.101556   -1.231503    0.320225
   25          1             0        4.991667   -1.853728    0.352877
   26          6             0        2.852527   -1.798114    0.520341
   27          1             0        2.753153   -2.865813    0.701366
   28          6             0       -1.476365    0.568219   -1.887309
   29          6             0       -1.571812   -1.658362   -1.407377
   30          8             0       -2.328153   -0.504461   -1.569687
   31          8             0       -2.077638   -2.741081   -1.268425
   32          8             0       -1.913715    1.639014   -2.209705
   33          6             0        0.658659    2.534649   -0.190900
   34          7             0        0.749472    3.650319   -0.501979
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3942776      0.2673910
0.2444898
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1867.3359161325 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
 HarFok:  IExCor= 402 AccDes= 0.00D+00 IRadAn=         4 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1011.05910939     A.U. after   15 cycles
            Convg  =    0.8468D-08             -V/T =  2.0093
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000980637    0.000798576    0.000162298
    2          6           0.000125974    0.001084266    0.001900690
    3          6          -0.000146551    0.000011018   -0.000284874
    4          6           0.000094129   -0.000043023    0.000495661
```

5	1	0.000042998	0.000107943	0.000018073
6	6	-0.000092847	-0.000048279	0.000536778
7	1	0.000151671	0.000113173	-0.000012250
8	6	-0.000894796	-0.002457682	0.000100312
9	1	0.000355142	-0.000075024	-0.000014756
10	6	0.000094592	0.000037829	-0.000051418
11	1	0.000014985	0.000008431	0.000049366
12	6	-0.000006846	-0.000007110	0.000175153
13	1	0.000020721	-0.000013855	-0.000008985
14	6	-0.000047780	0.000051666	-0.000060708
15	1	0.000017802	0.000008801	-0.000001591
16	6	0.000080517	-0.000057575	-0.000058186
17	1	0.000038896	-0.000024169	-0.000024145
18	6	-0.000022902	-0.000122249	-0.000164068
19	6	0.001418888	0.000297447	0.000083811
20	6	-0.000040359	0.000076774	-0.000092858
21	1	-0.000012069	-0.000018755	0.000059188
22	6	-0.000019140	0.000005268	0.000092866
23	1	-0.000027102	0.000001678	-0.000014694
24	6	0.000006577	0.000002085	0.000025848
25	1	-0.000009346	0.000007866	-0.000007137
26	6	0.000036022	-0.000062195	-0.000049739
27	1	-0.000019867	0.000026251	-0.000021002
28	6	-0.000257343	0.000063742	-0.000336609
29	6	-0.000208937	0.000012297	0.000027973
30	8	-0.000015183	0.000026043	0.000095642
31	8	0.000061294	0.000014843	0.000090367
32	8	0.000037199	-0.000162820	0.000253126
33	6	0.000059417	0.000583536	0.001238152
34	7	0.000144883	-0.000246798	-0.004202284

Cartesian Forces: Max 0.004202284 RMS 0.000596926

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Internal Forces: Max 0.004209619 RMS 0.000415281
Search for a saddle point.
Step number 3 out of a maximum of 195
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Swaping is turned off.
Update second derivatives using D2CorX and points 1 2 3
Eigenvalues --- -0.02413 0.00215 0.00740 0.00805
0.01149
Eigenvalues --- 0.01221 0.01481 0.01543 0.01607
0.01646
Eigenvalues --- 0.01748 0.01809 0.01903 0.01919
0.01946
Eigenvalues --- 0.02015 0.02105 0.02166 0.02222
0.02275

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02399   0.02475   0.02493   0.02514
0.02714
     Eigenvalues ---    0.02759   0.02770   0.02778   0.03432
0.04009
     Eigenvalues ---    0.05469   0.06599   0.06995   0.07517
0.08523
     Eigenvalues ---    0.10393   0.11109   0.11159   0.11193
0.11823
     Eigenvalues ---    0.11898   0.12501   0.12521   0.12652
0.12705
     Eigenvalues ---    0.12926   0.14238   0.16417   0.17474
0.18050
     Eigenvalues ---    0.19145   0.19178   0.19202   0.19398
0.19566
     Eigenvalues ---    0.19763   0.20290   0.20986   0.23495
0.23972
     Eigenvalues ---    0.25089   0.25139   0.26061   0.27941
0.28534
     Eigenvalues ---    0.29531   0.30086   0.30976   0.31764
0.33460
     Eigenvalues ---    0.34196   0.35307   0.35875   0.35904
0.36040
     Eigenvalues ---    0.36126   0.36226   0.36265   0.36292
0.36350
     Eigenvalues ---    0.37233   0.38031   0.39099   0.40157
0.40797
     Eigenvalues ---    0.41731   0.42418   0.42900   0.44742
0.47343
     Eigenvalues ---    0.47622   0.50294   0.50637   0.88539
0.89747
     Eigenvalues ---
1.375121000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
          1             -0.05292   0.02403   0.16531   0.01884
0.42773
                           R6        R7        R8        R9        R10
          1              0.15977  -0.05488  -0.03886  -0.05427
0.16166
                           R11       R12       R13       R14       R15
          1              0.01877  -0.00711   0.40535   0.15352  -
0.05429
                           R16       R17       R18       R19       R20
          1              0.27258  -0.00652  -0.09484   0.17162  -
0.00799
                           R21       R22       R23       R24       R25
          1             -0.02062  -0.00893   0.15631  -0.01137  -
0.05832
                           R26       R27       R28       R29       R30
          1              0.07662  -0.00028  -0.01469   0.00002
0.01606
                           R31       R32       R33       R34       R35
          1             -0.00011  -0.01536  -0.00021   0.02047
0.01800
                           R36       R37       R38       R39       R40
          1              0.01849  -0.00005  -0.01421   0.00006
0.01543
                           R41       R42       R43       R44       R45
          1             -0.00006  -0.01481  -0.00007   0.00268
0.00218
                           R46       R47       R48       A1        A2
          1             -0.00258   0.00205  -0.00056   0.02233  -
0.01178
                           A3        A4        A5        A6        A7
          1             -0.00962   0.04705   0.02069   0.01961
0.01873
                           A8        A9        A10       A11       A12
          1             -0.00477  -0.01321   0.02527   0.05221
0.02258
                           A13       A14       A15       A16       A17
```

This journal is © The Royal Society of Chemistry 2014

1	0.05434	0.03215	0.01641	0.04935	0.01317

	A18	A19	A20	A21	A22
1	0.02544	-0.00624	0.00602	0.00022	0.00072

	A23	A24	A25	A26	A27
1	0.00276	-0.00347	-0.00242	0.00099	0.00145

	A28	A29	A30	A31	A32
1	0.00471	-0.00594	0.00122	0.01909	-0.01411

	A33	A34	A35	A36	A37
1	-0.00425	0.02370	-0.01353	-0.00941	-0.00631

	A38	A39	A40	A41	A42
1	0.00620	0.00007	0.00110	0.00219	-0.00329

	A43	A44	A45	A46	A47
1	-0.00228	0.00050	0.00179	0.00480	-0.00580

	A48	A49	A50	A51	A52
1	0.00095	-0.00335	0.00417	-0.00083	-0.00497

	A53	A54	A55	A56	A57
1	0.00238	0.00269	-0.01385	-0.00369	0.01613

	D1	D2	D3	D4	D5
1	0.16923	-0.03491	0.15458	-0.04956	-0.00461

	D6	D7	D8	D9	D10
1	-0.01312	0.00918	0.00066	0.01345	0.01444

	D11	D12	D13	D14	D15
1	-0.00293	-0.00193	-0.16763	-0.15522	0.03490

	D16	D17	D18	D19	D20
1	0.04731	0.04311	-0.15827	0.05254	-0.14884

	D21	D22	D23	D24	D25
1	0.00094	0.00264	-0.00990	-0.00820	0.15933

	D26	D27	D28	D29	D30
1	0.15067	-0.04392	-0.05258	-0.01131	0.16549

	D31	D32	D33	D34	D35
1	-0.17588	0.00092	-0.13697	-0.14325	0.02558

	D36	D37	D38	D39	D40
1	0.01930	-0.02673	-0.02546	0.14450	0.14576

	D41	D42	D43	D44	D45

```
          1              0.00054   0.00141   0.00158   0.00245  -
0.00126
                           D46       D47       D48       D49       D50
          1             -0.00002  -0.00036   0.00088  -0.00113  -
0.00288
                           D51       D52       D53       D54       D55
          1              0.00008  -0.00168   0.00198  -0.00957
0.00965
                           D56       D57       D58       D59       D60
          1             -0.00190   0.01060   0.00742   0.00047  -
0.00271
                           D61       D62       D63       D64       D65
          1             -0.00989  -0.01186   0.00415   0.00218
0.00067
                           D66       D67       D68       D69       D70
          1             -0.00085  -0.00139  -0.00290   0.00155  -
0.00045
                           D71       D72       D73       D74       D75
          1              0.00003  -0.00197   0.00061   0.00390  -
0.00139
                           D76       D77       D78       D79       D80
          1              0.00190   0.04541   0.04429  -0.04585  -
0.04014
 RFO step:  Lambda0=1.755848344D-05 Lambda=-3.65728997D-04.
 Linear search not attempted -- option 19 set.
 Maximum step size (   0.300) exceeded in Quadratic search.
    -- Step size scaled by   0.896
 Iteration  1 RMS(Cart)=  0.02283046 RMS(Int)=  0.00025932
 Iteration  2 RMS(Cart)=  0.00033520 RMS(Int)=  0.00008478
 Iteration  3 RMS(Cart)=  0.00000006 RMS(Int)=  0.00008478
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.74094   0.00060   0.00000  -0.00086  -0.00091
2.74003
    R2        2.68568   0.00005   0.00000  -0.00085  -0.00085
2.68483
    R3        5.38905   0.00055   0.00000   0.06444   0.06457
5.45361
    R4        2.66924  -0.00010   0.00000   0.00046   0.00047
2.66971
    R5        4.33466   0.00115   0.00000   0.10634   0.10640
4.44106
    R6        4.79994  -0.00049   0.00000   0.07837   0.07839
4.87833
    R7        2.74801   0.00049   0.00000   0.00002   0.00003
2.74803
    R8        2.70688   0.00263   0.00000   0.00168   0.00174
2.70862
    R9        2.72484   0.00020   0.00000   0.00686   0.00687
2.73171
```

This journal is © The Royal Society of Chemistry 2014

R10	5.24335	0.00037	0.00000	-0.05309	-0.05315
5.19020					
R11	2.66808	-0.00012	0.00000	-0.00233	-0.00233
2.66575					
R12	2.05712	0.00012	0.00000	0.00029	0.00029
2.05741					
R13	4.00383	0.00001	0.00000	-0.10700	-0.10709
3.89673					
R14	4.61188	-0.00001	0.00000	-0.07734	-0.07734
4.53455					
R15	2.72990	0.00015	0.00000	0.00603	0.00604
2.73595					
R16	4.82649	-0.00020	0.00000	-0.10301	-0.10301
4.72348					
R17	2.04625	0.00018	0.00000	0.00120	0.00118
2.04743					
R18	2.66664	0.00058	0.00000	0.00442	0.00446
2.67110					
R19	5.05889	0.00025	0.00000	-0.03611	-0.03612
5.02277					
R20	2.81429	0.00007	0.00000	0.00920	0.00924
2.82353					
R21	5.13333	-0.00050	0.00000	-0.00544	-0.00537
5.12796					
R22	2.04278	0.00044	0.00000	-0.00003	-0.00003
2.04274					
R23	5.25269	0.00118	0.00000	0.05499	0.05498
5.30767					
R24	2.79709	0.00031	0.00000	-0.00894	-0.00892
2.78817					
R25	5.27498	0.00004	0.00000	0.01883	0.01882
5.29380					
R26	5.39952	0.00065	0.00000	0.12268	0.12256
5.52208					
R27	2.05237	-0.00005	0.00000	-0.00009	-0.00009
2.05228					
R28	2.61682	0.00003	0.00000	0.00002	0.00002
2.61684					
R29	2.05291	-0.00002	0.00000	-0.00003	-0.00003
2.05288					
R30	2.66628	-0.00009	0.00000	-0.00068	-0.00068
2.66560					
R31	2.05286	-0.00001	0.00000	-0.00002	-0.00002
2.05284					
R32	2.61631	0.00002	0.00000	0.00112	0.00111
2.61742					
R33	2.05355	-0.00002	0.00000	-0.00011	-0.00011
2.05344					
R34	2.68080	-0.00003	0.00000	-0.00016	-0.00011
2.68069					
R35	2.66551	-0.00003	0.00000	-0.00174	-0.00174
2.66377					

This journal is © The Royal Society of Chemistry 2014

R36	2.66814	-0.00007	0.00000	0.00042	0.00042
2.66856					
R37	2.05292	-0.00006	0.00000	-0.00018	-0.00018
2.05274					
R38	2.61960	0.00002	0.00000	-0.00013	-0.00013
2.61947					
R39	2.05313	-0.00002	0.00000	-0.00004	-0.00004
2.05309					
R40	2.66536	-0.00003	0.00000	-0.00039	-0.00039
2.66497					
R41	2.05323	-0.00001	0.00000	-0.00003	-0.00003
2.05320					
R42	2.61928	-0.00007	0.00000	0.00091	0.00091
2.62018					
R43	2.05505	-0.00002	0.00000	0.00001	0.00001
2.05506					
R44	2.65711	0.00018	0.00000	0.00805	0.00797
2.66508					
R45	2.26910	-0.00023	0.00000	0.00007	0.00007
2.26917					
R46	2.62521	-0.00003	0.00000	-0.00684	-0.00691
2.61830					
R47	2.27353	0.00006	0.00000	-0.00019	-0.00019
2.27334					
R48	2.19545	0.00421	0.00000	0.00345	0.00345
2.19890					
A1	2.02710	-0.00028	0.00000	0.00028	0.00030
2.02739					
A2	2.16599	0.00020	0.00000	0.00018	0.00012
2.16612					
A3	2.08782	0.00008	0.00000	0.00031	0.00028
2.08811					
A4	2.06855	0.00009	0.00000	0.00345	0.00334
2.07189					
A5	2.06701	0.00039	0.00000	0.00118	0.00109
2.06810					
A6	2.05148	-0.00046	0.00000	0.00276	0.00278
2.05425					
A7	2.03741	0.00033	0.00000	-0.00110	-0.00112
2.03629					
A8	2.08758	-0.00009	0.00000	0.00029	0.00030
2.08788					
A9	2.15460	-0.00023	0.00000	0.00036	0.00035
2.15495					
A10	2.04535	0.00002	0.00000	-0.00572	-0.00601
2.03935					
A11	2.05999	-0.00006	0.00000	-0.00789	-0.00807
2.05192					
A12	2.05388	0.00003	0.00000	-0.00544	-0.00574
2.04814					
A13	2.17190	-0.00002	0.00000	-0.01284	-0.01329
2.15861					

This journal is © The Royal Society of Chemistry 2014

A14	2.06435	-0.00016	0.00000	-0.00793	-0.00846
2.05589					
A15	1.86271	0.00014	0.00000	-0.00727	-0.00739
1.85532					
A16	2.20371	0.00015	0.00000	0.00502	0.00452
2.20823					
A17	1.87231	-0.00029	0.00000	0.00609	0.00605
1.87836					
A18	2.08339	0.00011	0.00000	0.00922	0.00888
2.09227					
A19	2.08967	0.00002	0.00000	0.00006	0.00005
2.08972					
A20	2.08977	-0.00006	0.00000	-0.00050	-0.00048
2.08929					
A21	2.10370	0.00004	0.00000	0.00042	0.00041
2.10412					
A22	2.08765	-0.00004	0.00000	-0.00016	-0.00017
2.08748					
A23	2.10641	0.00003	0.00000	-0.00009	-0.00009
2.10632					
A24	2.08907	0.00001	0.00000	0.00027	0.00027
2.08934					
A25	2.09008	0.00001	0.00000	0.00020	0.00021
2.09028					
A26	2.10030	-0.00003	0.00000	-0.00004	-0.00005
2.10025					
A27	2.09273	0.00001	0.00000	-0.00016	-0.00016
2.09257					
A28	2.09348	0.00007	0.00000	0.00005	0.00005
2.09352					
A29	2.08361	-0.00008	0.00000	0.00000	0.00000
2.08362					
A30	2.10607	0.00001	0.00000	-0.00004	-0.00004
2.10603					
A31	2.03517	0.00015	0.00000	-0.00074	-0.00071
2.03447					
A32	2.15516	-0.00014	0.00000	0.00051	0.00048
2.15564					
A33	2.08877	-0.00001	0.00000	-0.00012	-0.00014
2.08863					
A34	2.02904	-0.00004	0.00000	-0.00032	-0.00033
2.02872					
A35	2.16601	0.00004	0.00000	0.00016	0.00014
2.16615					
A36	2.08599	0.00001	0.00000	0.00063	0.00063
2.08662					
A37	2.08966	0.00001	0.00000	0.00015	0.00015
2.08981					
A38	2.09293	-0.00003	0.00000	-0.00067	-0.00067
2.09226					
A39	2.10042	0.00002	0.00000	0.00054	0.00053
2.10095					

This journal is © The Royal Society of Chemistry 2014

A40	2.08870	-0.00004	0.00000	-0.00018	-0.00019	2.08851
A41	2.10435	0.00004	0.00000	0.00003	0.00003	2.10438
A42	2.09014	0.00000	0.00000	0.00016	0.00015	2.09029
A43	2.09117	0.00002	0.00000	0.00003	0.00003	2.09120
A44	2.09786	-0.00004	0.00000	0.00012	0.00013	2.09798
A45	2.09416	0.00002	0.00000	-0.00015	-0.00015	2.09400
A46	2.09572	0.00003	0.00000	0.00002	0.00003	2.09575
A47	2.08396	-0.00004	0.00000	0.00028	0.00028	2.08424
A48	2.10335	0.00001	0.00000	-0.00032	-0.00032	2.10303
A49	1.88223	0.00007	0.00000	-0.00179	-0.00177	1.88046
A50	2.28293	0.00004	0.00000	0.00497	0.00495	2.28788
A51	2.11802	-0.00011	0.00000	-0.00318	-0.00319	2.11483
A52	1.88744	-0.00003	0.00000	0.00156	0.00162	1.88907
A53	2.26371	-0.00009	0.00000	-0.00553	-0.00556	2.25815
A54	2.13188	0.00011	0.00000	0.00390	0.00387	2.13574
A55	1.90736	0.00011	0.00000	0.00066	0.00059	1.90795
A56	3.16262	0.00011	0.00000	-0.00209	-0.00209	3.16053
A57	3.12905	-0.00014	0.00000	-0.00696	-0.00696	3.12209
D1	-0.56707	0.00016	0.00000	0.01128	0.01131	-0.55577
D2	3.04222	0.00024	0.00000	-0.00628	-0.00621	3.03602
D3	2.64740	0.00005	0.00000	-0.00103	-0.00103	2.64637
D4	-0.02649	0.00013	0.00000	-0.01858	-0.01854	-0.04504
D5	-0.01888	0.00004	0.00000	-0.01940	-0.01943	-0.03831
D6	-3.07249	-0.00008	0.00000	-0.01401	-0.01404	-3.08652
D7	3.05330	0.00016	0.00000	-0.00769	-0.00769	3.04562
D8	-0.00031	0.00003	0.00000	-0.00230	-0.00229	-0.00260

This journal is © The Royal Society of Chemistry 2014

D9	-0.05108	0.00006	0.00000	0.01143	0.01146	-0.03963
D10	3.10002	0.00005	0.00000	0.01363	0.01366	3.11368
D11	-3.11741	-0.00005	0.00000	-0.00127	-0.00128	-3.11870
D12	0.03369	-0.00005	0.00000	0.00092	0.00091	0.03461
D13	0.56436	-0.00022	0.00000	-0.00712	-0.00713	0.55723
D14	-2.64800	-0.00008	0.00000	0.00061	0.00061	-2.64739
D15	-3.04079	-0.00007	0.00000	0.00986	0.00979	-3.03100
D16	0.03004	0.00007	0.00000	0.01759	0.01754	0.04757
D17	-3.05848	-0.00021	0.00000	-0.01740	-0.01735	-3.07582
D18	0.60859	-0.00021	0.00000	0.02131	0.02125	0.62984
D19	-0.00857	-0.00006	0.00000	-0.02302	-0.02298	-0.03155
D20	-2.62469	-0.00006	0.00000	0.01568	0.01561	-2.60908
D21	-0.03423	0.00001	0.00000	0.00148	0.00147	-0.03276
D22	3.11449	0.00004	0.00000	0.00005	0.00005	3.11454
D23	-3.08164	-0.00016	0.00000	0.00733	0.00734	-3.07430
D24	0.06709	-0.00013	0.00000	0.00590	0.00591	0.07300
D25	-0.61121	0.00013	0.00000	-0.01697	-0.01689	-0.62811
D26	2.62793	0.00013	0.00000	-0.01269	-0.01263	2.61530
D27	3.05843	0.00013	0.00000	0.02200	0.02198	3.08041
D28	0.01439	0.00013	0.00000	0.02628	0.02624	0.04063
D29	-0.07765	-0.00014	0.00000	-0.07173	-0.07155	-0.14921
D30	2.53856	-0.00019	0.00000	-0.02929	-0.02909	2.50947
D31	-2.58564	-0.00003	0.00000	-0.02689	-0.02696	-2.61261
D32	0.03057	-0.00008	0.00000	0.01554	0.01550	0.04607
D33	-2.66800	0.00012	0.00000	0.02973	0.02971	-2.63830
D34	0.49285	0.00006	0.00000	0.03351	0.03346	0.52631

This journal is © The Royal Society of Chemistry 2014

D35	-0.11410	0.00006	0.00000	-0.01395	-0.01387	-0.12798
D36	3.04675	0.00000	0.00000	-0.01017	-0.01012	3.03663
D37	0.06163	0.00006	0.00000	-0.01270	-0.01271	0.04892
D38	-3.07938	0.00013	0.00000	-0.00783	-0.00786	-3.08724
D39	2.72068	0.00005	0.00000	0.02485	0.02493	2.74560
D40	-0.42033	0.00011	0.00000	0.02972	0.02978	-0.39055
D41	3.11967	0.00001	0.00000	-0.00037	-0.00037	3.11930
D42	-0.03301	0.00003	0.00000	0.00129	0.00130	-0.03171
D43	-0.01233	0.00001	0.00000	0.00184	0.00185	-0.01048
D44	3.11817	0.00003	0.00000	0.00351	0.00352	3.12169
D45	-3.12974	-0.00003	0.00000	-0.00207	-0.00207	-3.13181
D46	-0.00174	0.00001	0.00000	-0.00212	-0.00212	-0.00386
D47	0.00076	-0.00001	0.00000	-0.00040	-0.00040	0.00036
D48	3.12875	0.00003	0.00000	-0.00045	-0.00045	3.12830
D49	0.03553	-0.00003	0.00000	0.00072	0.00072	0.03624
D50	-3.11329	-0.00006	0.00000	0.00216	0.00216	-3.11113
D51	-3.11969	0.00001	0.00000	0.00067	0.00067	-3.11901
D52	0.01468	-0.00002	0.00000	0.00211	0.00211	0.01679
D53	0.02472	0.00014	0.00000	0.01146	0.01146	0.03618
D54	-3.04954	0.00000	0.00000	0.00412	0.00410	-3.04543
D55	3.07267	0.00014	0.00000	0.00740	0.00741	3.08008
D56	-0.00158	0.00000	0.00000	0.00006	0.00005	-0.00153
D57	3.07175	0.00000	0.00000	-0.00438	-0.00436	3.06739
D58	-0.08860	-0.00001	0.00000	-0.00511	-0.00509	-0.09369
D59	0.03055	-0.00001	0.00000	0.00006	0.00006	0.03061
D60	-3.12979	-0.00002	0.00000	-0.00067	-0.00067	-3.13047

```
   D61        0.06496  -0.00012   0.00000  -0.00840  -0.00841
0.05656
   D62       -3.09634  -0.00012   0.00000  -0.00778  -0.00779  -
3.10413
   D63        3.13362   0.00003   0.00000  -0.00046  -0.00046
3.13316
   D64       -0.02769   0.00002   0.00000   0.00015   0.00016  -
0.02753
   D65       -3.11364   0.00000   0.00000  -0.00030  -0.00030  -
3.11394
   D66        0.02836  -0.00003   0.00000  -0.00049  -0.00049
0.02787
   D67        0.00812  -0.00001   0.00000   0.00032   0.00032
0.00844
   D68       -3.13306  -0.00004   0.00000   0.00013   0.00012  -
3.13294
   D69        3.14103   0.00002   0.00000   0.00086   0.00086  -
3.14130
   D70        0.00076   0.00001   0.00000   0.00059   0.00059
0.00135
   D71       -0.00015   0.00000   0.00000   0.00066   0.00066
0.00051
   D72       -3.14042  -0.00001   0.00000   0.00040   0.00039  -
3.14003
   D73       -0.03033   0.00001   0.00000  -0.00039  -0.00038  -
0.03072
   D74        3.13022   0.00001   0.00000   0.00034   0.00035
3.13057
   D75        3.11258   0.00000   0.00000  -0.00066  -0.00066
3.11193
   D76       -0.01005   0.00000   0.00000   0.00008   0.00008  -
0.00997
   D77       -0.13601  -0.00004   0.00000   0.00362   0.00361  -
0.13239
   D78        3.00507  -0.00010   0.00000  -0.00069  -0.00066
3.00441
   D79        0.15521  -0.00002   0.00000   0.00625   0.00625
0.16146
   D80       -3.00389   0.00003   0.00000   0.00269   0.00269  -
3.00120
         Item               Value     Threshold  Converged?
 Maximum Force            0.004210     0.000450     NO
 RMS     Force            0.000415     0.000300     NO
 Maximum Displacement     0.129323     0.001800     NO
 RMS     Displacement     0.022896     0.001200     NO
 Predicted change in Energy=-1.885583D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.559141	1.131876	-0.758954
2	6	0	0.532579	0.441760	-1.417951
3	6	0	-0.562482	1.086700	0.661075
4	6	0	0.490292	0.319999	1.288349
5	1	0	0.454332	0.230894	2.372835
6	6	0	-0.012812	-1.603111	0.740046
7	1	0	0.749981	-2.064535	1.355764
8	6	0	-0.052056	-1.707728	-0.669017
9	1	0	0.713386	-2.130892	-1.304258
10	6	0	-1.623056	1.764030	-1.440367
11	1	0	-1.632859	1.780763	-2.526215
12	6	0	-2.637510	2.369268	-0.717756
13	1	0	-3.443922	2.872907	-1.243277
14	6	0	-2.640023	2.328540	0.692229
15	1	0	-3.448080	2.800503	1.243932
16	6	0	-1.626652	1.676399	1.375042
17	1	0	-1.638122	1.617452	2.460013
18	6	0	1.797191	0.341878	0.665724
19	6	0	1.823918	0.380957	-0.752045
20	6	0	3.059974	0.286066	-1.428288
21	1	0	3.083170	0.307751	-2.514086
22	6	0	4.237743	0.188761	-0.703831
23	1	0	5.188648	0.141961	-1.227240
24	6	0	4.211746	0.149792	0.705634
25	1	0	5.142343	0.073671	1.261236
26	6	0	3.003213	0.207044	1.382886
27	1	0	2.977010	0.167046	2.469326
28	6	0	-1.469173	-1.789213	-1.071572
29	6	0	-1.429795	-1.687231	1.206480
30	8	0	-2.254595	-1.666830	0.093366
31	8	0	-1.862402	-1.740507	2.327740
32	8	0	-1.975938	-1.936131	-2.150232
33	6	0	0.514892	0.342424	-2.847734
34	7	0	0.525340	0.260378	-4.008398

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.449962	0.000000			
3	C	1.420752	2.436690	0.000000		
4	C	2.439653	2.709367	1.445557	0.000000	
5	H	3.412770	3.797452	2.167126	1.088734	0.000000
6	C	3.166328	3.022564	2.746535	2.062062	2.499559
7	H	4.050047	3.744632	3.483594	2.399580	2.528010
8	C	2.885928	2.350106	3.136639	2.870035	3.642464
9	H	3.544339	2.581502	3.980361	3.574667	4.377917
10	C	1.412748	2.528965	2.449419	3.741304	4.605058
11	H	2.167287	2.776742	3.433111	4.603531	5.546093
12	C	2.419183	3.775582	2.802123	4.243478	4.866609

This journal is © The Royal Society of Chemistry 2014

13	H	3.404073	4.664069	3.888417	5.329588	5.937414
14	C	2.804996	4.251847	2.420602	3.766759	4.098731
15	H	3.891251	5.338065	3.406394	4.654637	4.806884
16	C	2.447452	3.739976	1.410656	2.515709	2.723155
17	H	3.429538	4.597042	2.162146	2.754329	2.511674
18	C	2.864631	2.439451	2.474437	1.447800	2.174814
19	C	2.498580	1.454196	2.861798	2.438336	3.415136
20	C	3.776426	2.532207	4.257774	3.739590	4.608790
21	H	4.126270	2.779386	4.896855	4.602356	5.549657
22	C	4.889029	3.781827	5.070644	4.246103	4.876663
23	H	5.851180	4.669607	6.126481	5.332395	5.948294
24	C	5.086342	4.258066	4.865494	3.770642	4.111483
25	H	6.140675	5.344479	5.825071	4.658647	4.820562
26	C	4.258305	3.742167	3.742858	2.517234	2.734476
27	H	4.884369	4.600178	4.079650	2.757149	2.525330
28	C	3.075492	3.017321	3.477790	3.722567	4.432228
29	C	3.545185	3.907832	2.957092	2.778922	2.930789
30	O	3.381386	3.807699	3.281382	3.593032	4.016917
31	O	4.413248	4.952617	3.529966	3.295631	3.042321
32	O	3.654537	3.533165	4.363349	4.795441	5.573181
33	C	2.477859	1.433339	3.745187	4.136217	5.222112
34	N	3.534756	2.596800	4.865198	5.297199	6.381696

		6	7	8	9	10
6	C	0.000000				
7	H	1.083454	0.000000			
8	C	1.413486	2.206878	0.000000		
9	H	2.232733	2.661101	1.080972	0.000000	
10	C	4.322583	5.301656	3.887946	4.543996	0.000000
11	H	4.974295	5.961040	4.256488	4.722191	1.086022
12	C	4.979359	5.952578	4.827923	5.641270	1.384772
13	H	5.978363	6.980126	5.728590	6.505761	2.141029
14	C	4.728891	5.588516	4.984178	5.926032	2.429168
15	H	5.607743	6.426882	5.959572	6.937559	3.407411
16	C	3.709836	4.432081	4.255566	5.210556	2.816774
17	H	3.996491	4.525420	4.833555	5.809424	3.903162
18	C	2.657934	2.713600	3.066290	3.342163	4.261013
19	C	3.088112	3.402444	2.808697	2.801358	3.777342
20	C	4.208642	4.314201	3.773120	3.370985	4.910732
21	H	4.881175	5.103650	4.158856	3.609229	5.042042
22	C	4.833508	4.635057	4.690444	4.261735	6.113340
23	H	5.828437	5.589481	5.585512	5.019936	7.005415
24	C	4.573919	4.160496	4.849748	4.634620	6.423083
25	H	5.445994	4.886073	5.820743	5.572927	7.478409
26	C	3.575795	3.199666	4.148654	4.234382	5.638912
27	H	3.881095	3.343596	4.747549	4.964318	6.244731
28	C	2.331863	3.300364	1.475435	2.221362	3.575643
29	C	1.494148	2.217220	2.327245	3.330746	4.353660
30	O	2.334063	3.283184	2.331111	3.313250	3.810771
31	O	2.441441	2.806114	3.501282	4.469731	5.151475
32	O	3.509768	4.442873	2.438747	2.825963	3.784128
33	C	4.115306	4.849548	3.044892	2.922159	2.927878
34	N	5.129320	5.850634	3.918967	3.614680	3.670335

This journal is © The Royal Society of Chemistry 2014

		11	12	13	14	15
11	H	0.000000				
12	C	2.150857	0.000000			
13	H	2.473592	1.086336	0.000000		
14	C	3.416551	1.410575	2.165357	0.000000	
15	H	4.306845	2.165920	2.488267	1.086316	0.000000
16	C	3.902657	2.425222	3.404364	1.385079	2.144388
17	H	4.988905	3.414999	4.307138	2.152792	2.480808
18	C	4.901439	5.068619	6.125329	4.861728	5.821686
19	C	4.129945	4.884557	5.848184	5.079939	6.134500
20	C	5.046012	6.107856	7.001902	6.415470	7.471139
21	H	4.940732	6.340570	7.127265	6.864327	7.936859
22	C	6.349765	7.212760	8.154975	7.336982	8.347866
23	H	7.134841	8.152865	9.054258	8.351861	9.368437
24	C	6.874905	7.339238	8.356007	7.189844	8.123359
25	H	7.947472	8.349388	9.371886	8.122403	9.012840
26	C	6.265048	6.395753	7.454469	6.068267	6.954460
27	H	6.986444	6.821298	7.895155	6.275444	7.051133
28	C	3.858433	4.333954	5.066012	4.630094	5.508459
29	C	5.099140	4.649349	5.554537	4.225581	4.920837
30	O	4.374318	4.134565	4.879583	4.058346	4.765005
31	O	6.001076	5.173595	6.044581	4.453845	4.930495
32	O	3.751582	4.585425	5.109246	5.167980	6.010262
33	C	2.604808	4.310747	4.964860	5.140962	6.203953
34	N	3.027583	5.027858	5.497840	6.032637	7.058844

		16	17	18	19	20
16	C	0.000000				
17	H	1.086632	0.000000			
18	C	3.742563	4.080188	0.000000		
19	C	4.255479	4.881798	1.418559	0.000000	
20	C	5.635259	6.242081	2.445940	1.412141	0.000000
21	H	6.259467	6.981946	3.430175	2.166994	1.086263
22	C	6.397336	6.824724	2.802752	2.421944	1.386163
23	H	7.454843	7.897955	3.889121	3.406514	2.142998
24	C	6.071699	6.281148	2.422512	2.807131	2.428739
25	H	6.957081	7.056559	3.408315	3.893542	3.408066
26	C	4.857439	4.969048	1.409606	2.445181	2.812857
27	H	4.966821	4.837686	2.162295	3.428208	3.900313
28	C	4.245137	4.909786	4.269529	3.956789	4.994716
29	C	3.373600	3.540576	3.850083	4.324335	5.567219
30	O	3.635132	4.094822	4.558451	4.641382	5.862924
31	O	3.555061	3.368039	4.526726	5.251156	6.514946
32	O	5.059637	5.830646	5.230242	4.665054	5.551555
33	C	4.919099	5.867993	3.740145	2.471224	2.914695
34	N	5.968049	6.954320	4.844757	3.507803	3.616904

		21	22	23	24	25
21	H	0.000000				
22	C	2.150400	0.000000			
23	H	2.473155	1.086447	0.000000		
24	C	3.415441	1.410244	2.165734	0.000000	
25	H	4.306745	2.166342	2.489844	1.086508	0.000000
26	C	3.899093	2.424621	3.404868	1.386542	2.146733

27	H	4.986528	3.414505	4.307734	2.153016	2.481303
28	C	5.215546	6.051157	6.933992	6.260274	7.254273
29	C	6.179759	6.268143	7.285103	5.954199	6.804173
30	O	6.260153	6.799206	7.772876	6.744520	7.688170
31	O	7.217847	7.079849	8.117813	6.565038	7.314036
32	O	5.546347	6.724364	7.516760	7.127024	8.145388
33	C	2.590091	4.298785	4.950776	5.131302	6.194285
34	N	2.962719	4.970637	5.430958	5.985309	7.008611

		26	27	28	29	30
26	C	0.000000				
27	H	1.087492	0.000000			
28	C	5.478288	6.011111	0.000000		
29	C	4.823998	4.945003	2.280674	0.000000	
30	O	5.728771	6.031417	1.410301	1.385545	0.000000
31	O	5.325403	5.203721	3.422327	1.203001	2.269729
32	O	6.470554	7.091923	1.200792	3.409947	2.276819
33	C	4.910012	5.862074	3.411032	4.933352	4.511900
34	N	5.933687	6.926782	4.099250	5.900059	5.316639

		31	32	33	34
31	O	0.000000			
32	O	4.483680	0.000000		
33	C	6.064294	3.447109	0.000000	
34	N	7.060560	3.812326	1.163607	0.000000

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.532329	0.759781	0.990090
2	6	0	0.595018	1.167978	0.174703
3	6	0	-0.648937	-0.632941	1.245555
4	6	0	0.336317	-1.490853	0.626768
5	1	0	0.212942	-2.563243	0.768549
6	6	0	-0.157738	-1.319906	-1.367921
7	1	0	0.545130	-2.078811	-1.690274
8	6	0	-0.087249	0.034114	-1.767425
9	1	0	0.718023	0.501813	-2.316330
10	6	0	-1.526921	1.643069	1.465953
11	1	0	-1.450404	2.705298	1.253216
12	6	0	-2.583884	1.148771	2.211669
13	1	0	-3.336578	1.832221	2.594389
14	6	0	-2.698789	-0.233297	2.469363
15	1	0	-3.539006	-0.605884	3.048411
16	6	0	-1.755059	-1.118038	1.974339
17	1	0	-1.853498	-2.186554	2.145661
18	6	0	1.688590	-0.985959	0.514674

This journal is © The Royal Society of Chemistry 2014

```
   19          6             0        1.828213    0.401377    0.253688
   20          6             0        3.111935    0.939732    0.016255
   21          1             0        3.221429    2.000269   -0.191684
   22          6             0        4.226617    0.117654    0.072096
   23          1             0        5.214934    0.540411   -0.085621
   24          6             0        4.088380   -1.261628    0.331437
   25          1             0        4.970476   -1.894636    0.372758
   26          6             0        2.831305   -1.811115    0.532248
   27          1             0        2.718420   -2.875882    0.722426
   28          6             0       -1.469321    0.524466   -1.929725
   29          6             0       -1.608530   -1.676754   -1.349445
   30          8             0       -2.342082   -0.520892   -1.563034
   31          8             0       -2.129478   -2.745175   -1.164243
   32          8             0       -1.891755    1.585723   -2.300110
   33          6             0        0.688733    2.541542   -0.224045
   34          7             0        0.789506    3.654255   -0.549155
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3922187      0.2666604
0.2440258
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1865.2635219896 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A)

Harris functional with IExCor= 402 diagonalized for initial guess.
ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
4 AccDes= 0.00D+00
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 4 IDoV=1
ScaDFX= 1.000000 1.000000 1.000000 1.000000
Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB+HF-LYP) = -1011.05928482 A.U. after 16 cycles
Convg = 0.4327D-08 -V/T = 2.0094
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000349452	0.000300104	0.000090004
2	6	0.000026489	0.000212571	0.001105465
3	6	-0.000296231	0.000217457	-0.000183938
4	6	-0.000181930	-0.000529856	0.000459906
5	1	0.000061125	0.000282070	0.000049661
6	6	0.000057537	0.000126178	0.000569210
7	1	0.000057246	-0.000194822	0.000060777
8	6	-0.000038324	-0.000223171	-0.000641764
9	1	0.000031914	-0.000074515	0.000001185
10	6	0.000039790	0.000005754	-0.000000078
11	1	-0.000007323	-0.000024176	0.000007964
12	6	-0.000026729	0.000023144	0.000023726

13	1	-0.000002361	-0.000006474	0.000000837
14	6	-0.000052016	0.000023890	-0.000055596
15	1	-0.000002791	-0.000002661	-0.000001857
16	6	0.000102286	-0.000032474	-0.000020101
17	1	0.000004627	0.000007429	-0.000002898
18	6	0.000381830	0.000013212	-0.000251928
19	6	0.000259583	-0.000096827	0.000081275
20	6	-0.000104395	-0.000001813	0.000017585
21	1	-0.000005502	0.000004525	-0.000003918
22	6	0.000050854	-0.000008187	0.000073934
23	1	-0.000002295	-0.000003421	-0.000001097
24	6	0.000068822	0.000007609	-0.000087319
25	1	0.000001931	-0.000000840	-0.000006295
26	6	-0.000116594	0.000038004	-0.000056466
27	1	-0.000005098	-0.000000548	-0.000003249
28	6	0.000006876	-0.000096812	-0.000051957
29	6	0.000035712	0.000031930	0.000166204
30	8	-0.000045657	-0.000018753	0.000003024
31	8	-0.000035022	-0.000037440	0.000083815
32	8	-0.000086975	-0.000013390	-0.000083600
33	6	0.000156078	0.000116988	-0.000977654
34	7	0.000015995	-0.000044688	-0.000364858

Cartesian Forces: Max 0.001105465 RMS 0.000214423

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Internal Forces: Max 0.001285895 RMS 0.000140247
Search for a saddle point.
Step number 4 out of a maximum of 195
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Swaping is turned off.
Update second derivatives using D2CorX and points 2 3 4
Eigenvalues --- -0.02417 0.00261 0.00740 0.00807
0.01149
Eigenvalues --- 0.01222 0.01482 0.01544 0.01607
0.01646
Eigenvalues --- 0.01752 0.01809 0.01905 0.01919
0.01948
Eigenvalues --- 0.02015 0.02106 0.02165 0.02222
0.02274
Eigenvalues --- 0.02401 0.02475 0.02493 0.02513
0.02714
Eigenvalues --- 0.02759 0.02770 0.02778 0.03430
0.04005
Eigenvalues --- 0.05468 0.06598 0.06986 0.07500
0.08511
Eigenvalues --- 0.10379 0.11088 0.11156 0.11193
0.11822

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.11898   0.12501   0.12521   0.12651
0.12704
     Eigenvalues ---    0.12925   0.14223   0.16411   0.17464
0.18039
     Eigenvalues ---    0.19144   0.19175   0.19200   0.19397
0.19563
     Eigenvalues ---    0.19761   0.20279   0.20984   0.23488
0.23970
     Eigenvalues ---    0.25085   0.25138   0.26055   0.27934
0.28527
     Eigenvalues ---    0.29527   0.30084   0.30952   0.31751
0.33457
     Eigenvalues ---    0.34193   0.35306   0.35874   0.35904
0.36040
     Eigenvalues ---    0.36126   0.36225   0.36265   0.36292
0.36350
     Eigenvalues ---    0.37231   0.38022   0.39099   0.40153
0.40789
     Eigenvalues ---    0.41730   0.42417   0.42888   0.44735
0.47342
     Eigenvalues ---    0.47621   0.50294   0.50637   0.88539
0.89747
     Eigenvalues ---
1.375131000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
          1            -0.05235   0.02414   0.15942   0.01874
0.41770
                           R6        R7        R8        R9        R10
          1             0.15329  -0.05457  -0.03896  -0.05499
0.16583
                           R11       R12       R13       R14       R15
          1             0.01892  -0.00656   0.41425   0.15880  -
0.05483
                           R16       R17       R18       R19       R20
          1             0.27908  -0.00638  -0.09524   0.17487  -
0.00929
                           R21       R22       R23       R24       R25
          1            -0.02053  -0.00909   0.15182  -0.01004  -
0.05952
                           R26       R27       R28       R29       R30
          1             0.06807  -0.00028  -0.01466   0.00002
0.01605
                           R31       R32       R33       R34       R35
          1            -0.00011  -0.01543  -0.00021   0.02053
0.01814
                           R36       R37       R38       R39       R40
          1             0.01842  -0.00005  -0.01419   0.00006
0.01543
                           R41       R42       R43       R44       R45
          1            -0.00006  -0.01490  -0.00007   0.00240
0.00212
                           R46       R47       R48       A1        A2
          1            -0.00241   0.00205  -0.00061   0.02217  -
0.01182
                           A3        A4        A5        A6        A7
          1            -0.00963   0.04632   0.01910   0.01769
0.01903
                           A8        A9        A10       A11       A12
          1            -0.00482  -0.01335   0.02874   0.05455
0.02615
                           A13       A14       A15       A16       A17
          1             0.05798   0.03623   0.01901   0.04644
0.01065
                           A18       A19       A20       A21       A22
          1             0.02184  -0.00623   0.00605   0.00017
0.00070
                           A23       A24       A25       A26       A27
          1             0.00279  -0.00348  -0.00242   0.00097
0.00146
```

This journal is © The Royal Society of Chemistry 2014

	A28	A29	A30	A31	A32
1	0.00472	-0.00597	0.00124	0.01922	-0.01417

	A33	A34	A35	A36	A37
1	-0.00423	0.02375	-0.01364	-0.00947	-0.00631

	A38	A39	A40	A41	A42
1	0.00625	0.00003	0.00108	0.00222	-0.00330

	A43	A44	A45	A46	A47
1	-0.00228	0.00048	0.00180	0.00479	-0.00583

	A48	A49	A50	A51	A52
1	0.00098	-0.00234	0.00333	-0.00099	-0.00596

	A53	A54	A55	A56	A57
1	0.00322	0.00287	-0.01383	-0.00355	0.01627

	D1	D2	D3	D4	D5
1	0.16804	-0.03443	0.15447	-0.04800	-0.00261

	D6	D7	D8	D9	D10
1	-0.01183	0.01017	0.00095	0.01220	0.01298

	D11	D12	D13	D14	D15
1	-0.00284	-0.00206	-0.16691	-0.15531	0.03424

	D16	D17	D18	D19	D20
1	0.04585	0.04349	-0.15915	0.05369	-0.14894

	D21	D22	D23	D24	D25
1	0.00076	0.00268	-0.01097	-0.00904	0.15968

	D26	D27	D28	D29	D30
1	0.15049	-0.04488	-0.05407	-0.00768	0.16637

	D31	D32	D33	D34	D35
1	-0.17371	0.00034	-0.13878	-0.14509	0.02616

	D36	D37	D38	D39	D40
1	0.01985	-0.02602	-0.02498	0.14267	0.14370

	D41	D42	D43	D44	D45
1	0.00056	0.00128	0.00139	0.00211	-0.00110

	D46	D47	D48	D49	D50
1	0.00021	-0.00036	0.00095	-0.00121	-0.00318

	D51	D52	D53	D54	D55
1	0.00007	-0.00190	0.00065	-0.01017	0.00878

	D56	D57	D58	D59	D60

```
          1             -0.00203   0.01129   0.00804   0.00057  -
0.00269
                           D61       D62       D63       D64       D65
          1             -0.00894  -0.01086   0.00414   0.00222
0.00068
                           D66       D67       D68       D69       D70
          1             -0.00076  -0.00132  -0.00276   0.00146  -
0.00057
                           D71       D72       D73       D74       D75
          1              0.00001  -0.00202   0.00064   0.00400  -
0.00139
                           D76       D77       D78       D79       D80
          1              0.00197   0.04497   0.04407  -0.04637  -
0.04058
 RFO step:  Lambda0=6.260057447D-07 Lambda=-2.64338269D-05.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.00394970 RMS(Int)=  0.00000764
 Iteration  2 RMS(Cart)=  0.00000916 RMS(Int)=  0.00000419
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000419
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.74003   0.00025   0.00000  -0.00034  -0.00035
2.73968
    R2        2.68483   0.00005   0.00000  -0.00003  -0.00003
2.68480
    R3        5.45361   0.00012   0.00000   0.01273   0.01274
5.46635
    R4        2.66971  -0.00003   0.00000   0.00008   0.00008
2.66979
    R5        4.44106   0.00016   0.00000   0.02309   0.02308
4.46414
    R6        4.87833  -0.00021   0.00000   0.01767   0.01767
4.89600
    R7        2.74803   0.00008   0.00000  -0.00063  -0.00063
2.74740
    R8        2.70862   0.00129   0.00000   0.00407   0.00407
2.71269
    R9        2.73171   0.00038   0.00000   0.00227   0.00227
2.73398
   R10        5.19020   0.00028   0.00000  -0.00320  -0.00320
5.18700
   R11        2.66575  -0.00005   0.00000  -0.00044  -0.00044
2.66531
   R12        2.05741   0.00002   0.00000   0.00011   0.00011
2.05752
   R13        3.89673  -0.00016   0.00000  -0.01454  -0.01454
3.88219
   R14        4.53455   0.00012   0.00000  -0.00348  -0.00349
4.53106
   R15        2.73595   0.00043   0.00000   0.00215   0.00215
2.73810
```

This journal is © The Royal Society of Chemistry 2014

R16	4.72348	0.00000	0.00000	-0.00540	-0.00540
4.71808					
R17	2.04743	0.00013	0.00000	0.00068	0.00068
2.04811					
R18	2.67110	0.00069	0.00000	0.00224	0.00224
2.67334					
R19	5.02277	-0.00002	0.00000	-0.00671	-0.00672
5.01605					
R20	2.82353	0.00002	0.00000	0.00166	0.00166
2.82519					
R21	5.12796	-0.00012	0.00000	0.00134	0.00135
5.12931					
R22	2.04274	0.00011	0.00000	0.00003	0.00003
2.04277					
R23	5.30767	0.00019	0.00000	0.01032	0.01032
5.31799					
R24	2.78817	0.00013	0.00000	-0.00145	-0.00145
2.78672					
R25	5.29380	0.00008	0.00000	0.00670	0.00670
5.30050					
R26	5.52208	0.00010	0.00000	0.02499	0.02499
5.54707					
R27	2.05228	-0.00001	0.00000	-0.00002	-0.00002
2.05226					
R28	2.61684	0.00000	0.00000	-0.00007	-0.00007
2.61677					
R29	2.05288	0.00000	0.00000	-0.00001	-0.00001
2.05287					
R30	2.66560	-0.00003	0.00000	-0.00007	-0.00007
2.66553					
R31	2.05284	0.00000	0.00000	0.00000	0.00000
2.05284					
R32	2.61742	0.00009	0.00000	0.00035	0.00035
2.61776					
R33	2.05344	0.00000	0.00000	0.00000	0.00000
2.05344					
R34	2.68069	-0.00008	0.00000	-0.00032	-0.00032
2.68037					
R35	2.66377	-0.00008	0.00000	-0.00050	-0.00050
2.66327					
R36	2.66856	-0.00006	0.00000	0.00009	0.00009
2.66865					
R37	2.05274	0.00000	0.00000	-0.00001	-0.00001
2.05273					
R38	2.61947	0.00004	0.00000	-0.00002	-0.00002
2.61945					
R39	2.05309	0.00000	0.00000	-0.00001	-0.00001
2.05307					
R40	2.66497	-0.00008	0.00000	-0.00019	-0.00019
2.66479					
R41	2.05320	0.00000	0.00000	0.00000	0.00000
2.05320					

This journal is © The Royal Society of Chemistry 2014

R42	2.62018	0.00006	0.00000	0.00030	0.00030
2.62049					
R43	2.05506	0.00000	0.00000	0.00001	0.00001
2.05507					
R44	2.66508	0.00017	0.00000	0.00162	0.00162
2.66670					
R45	2.26917	0.00011	0.00000	0.00025	0.00025
2.26942					
R46	2.61830	0.00013	0.00000	-0.00067	-0.00068
2.61762					
R47	2.27334	0.00009	0.00000	0.00001	0.00001
2.27335					
R48	2.19890	0.00037	0.00000	0.00032	0.00032
2.19922					
A1	2.02739	-0.00009	0.00000	-0.00014	-0.00014
2.02725					
A2	2.16612	0.00002	0.00000	-0.00014	-0.00014
2.16597					
A3	2.08811	0.00007	0.00000	0.00039	0.00039
2.08850					
A4	2.07189	0.00010	0.00000	0.00219	0.00218
2.07407					
A5	2.06810	0.00018	0.00000	0.00062	0.00061
2.06872					
A6	2.05425	-0.00028	0.00000	-0.00074	-0.00074
2.05351					
A7	2.03629	0.00011	0.00000	0.00040	0.00040
2.03669					
A8	2.08788	-0.00008	0.00000	-0.00034	-0.00034
2.08754					
A9	2.15495	-0.00002	0.00000	-0.00007	-0.00008
2.15488					
A10	2.03935	0.00000	0.00000	-0.00237	-0.00239
2.03696					
A11	2.05192	-0.00011	0.00000	-0.00163	-0.00164
2.05028					
A12	2.04814	0.00006	0.00000	-0.00180	-0.00183
2.04631					
A13	2.15861	0.00001	0.00000	-0.00283	-0.00285
2.15575					
A14	2.05589	-0.00010	0.00000	-0.00236	-0.00238
2.05351					
A15	1.85532	0.00005	0.00000	-0.00134	-0.00135
1.85397					
A16	2.20823	0.00003	0.00000	0.00054	0.00053
2.20875					
A17	1.87836	-0.00014	0.00000	0.00086	0.00086
1.87923					
A18	2.09227	0.00006	0.00000	0.00151	0.00150
2.09377					
A19	2.08972	0.00000	0.00000	-0.00012	-0.00012
2.08960					

This journal is © The Royal Society of Chemistry 2014

A20	2.08929	-0.00001	0.00000	-0.00012	-0.00012
2.08917					
A21	2.10412	0.00001	0.00000	0.00024	0.00024
2.10436					
A22	2.08748	0.00001	0.00000	0.00009	0.00009
2.08757					
A23	2.10632	-0.00003	0.00000	-0.00018	-0.00018
2.10614					
A24	2.08934	0.00002	0.00000	0.00010	0.00010
2.08944					
A25	2.09028	-0.00001	0.00000	-0.00003	-0.00003
2.09025					
A26	2.10025	0.00001	0.00000	0.00012	0.00012
2.10037					
A27	2.09257	0.00000	0.00000	-0.00009	-0.00009
2.09249					
A28	2.09352	0.00003	0.00000	0.00015	0.00015
2.09367					
A29	2.08362	-0.00001	0.00000	0.00011	0.00011
2.08373					
A30	2.10603	-0.00002	0.00000	-0.00025	-0.00025
2.10578					
A31	2.03447	0.00000	0.00000	0.00010	0.00011
2.03457					
A32	2.15564	0.00000	0.00000	-0.00012	-0.00012
2.15551					
A33	2.08863	0.00000	0.00000	-0.00009	-0.00009
2.08854					
A34	2.02872	0.00009	0.00000	0.00034	0.00033
2.02905					
A35	2.16615	-0.00009	0.00000	-0.00030	-0.00031
2.16584					
A36	2.08662	0.00000	0.00000	0.00010	0.00010
2.08672					
A37	2.08981	-0.00002	0.00000	-0.00005	-0.00005
2.08976					
A38	2.09226	0.00003	0.00000	0.00004	0.00004
2.09231					
A39	2.10095	-0.00001	0.00000	0.00000	0.00000
2.10096					
A40	2.08851	0.00001	0.00000	0.00005	0.00005
2.08856					
A41	2.10438	-0.00003	0.00000	-0.00017	-0.00017
2.10421					
A42	2.09029	0.00001	0.00000	0.00012	0.00012
2.09041					
A43	2.09120	0.00001	0.00000	0.00006	0.00006
2.09125					
A44	2.09798	-0.00003	0.00000	-0.00003	-0.00003
2.09795					
A45	2.09400	0.00002	0.00000	-0.00002	-0.00002
2.09398					

This journal is © The Royal Society of Chemistry 2014

A46	2.09575	0.00003	0.00000	0.00017	0.00017	2.09592
A47	2.08424	-0.00002	0.00000	0.00000	0.00000	2.08424
A48	2.10303	-0.00001	0.00000	-0.00015	-0.00015	2.10287
A49	1.88046	0.00000	0.00000	-0.00024	-0.00024	1.88022
A50	2.28788	0.00005	0.00000	0.00103	0.00103	2.28891
A51	2.11483	-0.00005	0.00000	-0.00079	-0.00079	2.11404
A52	1.88907	-0.00007	0.00000	0.00012	0.00013	1.88919
A53	2.25815	0.00004	0.00000	-0.00063	-0.00063	2.25751
A54	2.13574	0.00003	0.00000	0.00051	0.00051	2.13625
A55	1.90795	0.00016	0.00000	0.00036	0.00036	1.90831
A56	3.16053	0.00005	0.00000	0.00031	0.00031	3.16084
A57	3.12209	0.00001	0.00000	0.00149	0.00149	3.12358
D1	-0.55577	0.00007	0.00000	0.00482	0.00482	-0.55094
D2	3.03602	0.00014	0.00000	0.00009	0.00009	3.03611
D3	2.64637	0.00002	0.00000	0.00269	0.00269	2.64906
D4	-0.04504	0.00009	0.00000	-0.00203	-0.00203	-0.04707
D5	-0.03831	0.00001	0.00000	-0.00381	-0.00381	-0.04212
D6	-3.08652	-0.00007	0.00000	-0.00362	-0.00362	-3.09014
D7	3.04562	0.00005	0.00000	-0.00180	-0.00180	3.04381
D8	-0.00260	-0.00002	0.00000	-0.00161	-0.00161	-0.00421
D9	-0.03963	0.00005	0.00000	0.00326	0.00326	-0.03636
D10	3.11368	0.00004	0.00000	0.00290	0.00290	3.11658
D11	-3.11870	0.00000	0.00000	0.00109	0.00109	-3.11761
D12	0.03461	0.00000	0.00000	0.00072	0.00072	0.03533
D13	0.55723	-0.00011	0.00000	-0.00509	-0.00509	0.55214
D14	-2.64739	-0.00002	0.00000	-0.00262	-0.00262	-2.65001

This journal is © The Royal Society of Chemistry 2014

D15	-3.03100	-0.00007	0.00000	-0.00006	-0.00006	-3.03106
D16	0.04757	0.00002	0.00000	0.00241	0.00241	0.04998
D17	-3.07582	-0.00018	0.00000	-0.00885	-0.00884	-3.08466
D18	0.62984	-0.00012	0.00000	0.00202	0.00202	0.63186
D19	-0.03155	-0.00010	0.00000	-0.00906	-0.00906	-0.04061
D20	-2.60908	-0.00004	0.00000	0.00181	0.00180	-2.60727
D21	-0.03276	0.00004	0.00000	0.00128	0.00128	-0.03148
D22	3.11454	0.00004	0.00000	0.00090	0.00090	3.11544
D23	-3.07430	-0.00005	0.00000	0.00147	0.00147	-3.07284
D24	0.07300	-0.00005	0.00000	0.00108	0.00108	0.07408
D25	-0.62811	0.00006	0.00000	-0.00234	-0.00233	-0.63044
D26	2.61530	0.00006	0.00000	-0.00110	-0.00110	2.61420
D27	3.08041	0.00014	0.00000	0.00877	0.00877	3.08918
D28	0.04063	0.00014	0.00000	0.01001	0.01001	0.05064
D29	-0.14921	-0.00002	0.00000	-0.01202	-0.01201	-0.16122
D30	2.50947	-0.00013	0.00000	-0.00532	-0.00531	2.50416
D31	-2.61261	0.00007	0.00000	-0.00229	-0.00229	-2.61490
D32	0.04607	-0.00003	0.00000	0.00441	0.00441	0.05048
D33	-2.63830	0.00008	0.00000	0.00564	0.00564	-2.63266
D34	0.52631	0.00002	0.00000	0.00542	0.00542	0.53173
D35	-0.12798	0.00003	0.00000	-0.00366	-0.00366	-0.13163
D36	3.03663	-0.00003	0.00000	-0.00388	-0.00388	3.03275
D37	0.04892	0.00002	0.00000	-0.00381	-0.00381	0.04511
D38	-3.08724	0.00004	0.00000	-0.00354	-0.00354	-3.09078
D39	2.74560	-0.00007	0.00000	0.00206	0.00207	2.74767
D40	-0.39055	-0.00006	0.00000	0.00233	0.00233	-0.38822

This journal is © The Royal Society of Chemistry 2014

D41	3.11930	0.00001	0.00000	0.00034	0.00034	3.11964
D42	-0.03171	0.00002	0.00000	0.00050	0.00050	-0.03121
D43	-0.01048	0.00000	0.00000	-0.00002	-0.00002	-0.01051
D44	3.12169	0.00001	0.00000	0.00014	0.00014	3.12183
D45	-3.13181	-0.00002	0.00000	-0.00067	-0.00067	-3.13248
D46	-0.00386	0.00000	0.00000	-0.00083	-0.00083	-0.00469
D47	0.00036	0.00000	0.00000	-0.00051	-0.00051	-0.00015
D48	3.12830	0.00001	0.00000	-0.00067	-0.00067	3.12764
D49	0.03624	-0.00002	0.00000	-0.00007	-0.00007	0.03618
D50	-3.11113	-0.00002	0.00000	0.00033	0.00032	-3.11081
D51	-3.11901	-0.00001	0.00000	-0.00022	-0.00022	-3.11924
D52	0.01679	-0.00001	0.00000	0.00017	0.00017	0.01696
D53	0.03618	0.00012	0.00000	0.00445	0.00445	0.04063
D54	-3.04543	0.00003	0.00000	0.00212	0.00212	-3.04331
D55	3.08008	0.00011	0.00000	0.00327	0.00327	3.08335
D56	-0.00153	0.00003	0.00000	0.00093	0.00093	-0.00060
D57	3.06739	-0.00004	0.00000	-0.00216	-0.00215	3.06523
D58	-0.09369	-0.00001	0.00000	-0.00150	-0.00150	-0.09519
D59	0.03061	-0.00003	0.00000	-0.00089	-0.00089	0.02972
D60	-3.13047	-0.00001	0.00000	-0.00024	-0.00024	-3.13070
D61	0.05656	-0.00008	0.00000	-0.00266	-0.00266	0.05390
D62	-3.10413	-0.00010	0.00000	-0.00272	-0.00272	-3.10685
D63	3.13316	0.00002	0.00000	-0.00011	-0.00011	3.13305
D64	-0.02753	0.00000	0.00000	-0.00017	-0.00017	-0.02770
D65	-3.11394	0.00000	0.00000	-0.00043	-0.00043	-3.11437
D66	0.02787	-0.00002	0.00000	-0.00064	-0.00064	0.02723

```
   D67        0.00844  -0.00002   0.00000  -0.00050  -0.00050
0.00794
   D68       -3.13294  -0.00004   0.00000  -0.00070  -0.00070  -
3.13364
   D69       -3.14130   0.00001   0.00000   0.00044   0.00044  -
3.14086
   D70        0.00135   0.00002   0.00000   0.00068   0.00068
0.00203
   D71        0.00051  -0.00001   0.00000   0.00024   0.00024
0.00075
   D72       -3.14003   0.00000   0.00000   0.00047   0.00047  -
3.13956
   D73       -0.03072   0.00001   0.00000   0.00009   0.00009  -
0.03063
   D74        3.13057  -0.00002   0.00000  -0.00057  -0.00057
3.13000
   D75        3.11193   0.00002   0.00000   0.00033   0.00033
3.11226
   D76       -0.00997  -0.00001   0.00000  -0.00033  -0.00033  -
0.01030
   D77       -0.13239  -0.00002   0.00000   0.00140   0.00140  -
0.13100
   D78        3.00441  -0.00003   0.00000   0.00117   0.00117
3.00558
   D79        0.16146   0.00000   0.00000   0.00139   0.00139
0.16285
   D80       -3.00120   0.00005   0.00000   0.00157   0.00157  -
2.99962
         Item               Value     Threshold  Converged?
 Maximum Force            0.001286     0.000450     NO
 RMS     Force            0.000140     0.000300     YES
 Maximum Displacement     0.018126     0.001800     NO
 RMS     Displacement     0.003951     0.001200     NO
 Predicted change in Energy=-1.294469D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.559666    1.133977   -0.760879
    2          6             0        0.534120    0.447920   -1.420283
    3          6             0       -0.563866    1.085857    0.659037
    4          6             0        0.488167    0.315907    1.286345
    5          1             0        0.453730    0.233405    2.371460
    6          6             0       -0.011191   -1.601446    0.743369
    7          1             0        0.751054   -2.066301    1.357813
    8          6             0       -0.053202   -1.712439   -0.666317
    9          1             0        0.712736   -2.134062   -1.302010
```

10	6	0	-1.623226	1.766983	-1.442146
11	1	0	-1.632404	1.784804	-2.527970
12	6	0	-2.638078	2.371126	-0.719252
13	1	0	-3.444448	2.875188	-1.244419
14	6	0	-2.640798	2.328814	0.690649
15	1	0	-3.448786	2.800437	1.242741
16	6	0	-1.627774	1.675359	1.373091
17	1	0	-1.639918	1.615147	2.457987
18	6	0	1.796492	0.340652	0.664178
19	6	0	1.824297	0.382060	-0.753335
20	6	0	3.060762	0.287416	-1.428969
21	1	0	3.084609	0.310801	-2.514714
22	6	0	4.238036	0.188269	-0.703975
23	1	0	5.189210	0.141259	-1.226861
24	6	0	4.211002	0.147965	0.705335
25	1	0	5.141126	0.070822	1.261586
26	6	0	3.001831	0.204927	1.381797
27	1	0	2.974917	0.163355	2.468166
28	6	0	-1.470070	-1.794018	-1.066906
29	6	0	-1.428336	-1.688247	1.211635
30	8	0	-2.254276	-1.670487	0.099766
31	8	0	-1.858932	-1.741727	2.333665
32	8	0	-1.979310	-1.941952	-2.144407
33	6	0	0.518618	0.350901	-2.852412
34	7	0	0.530718	0.269971	-4.013307

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.449778	0.000000			
3	C	1.420737	2.436413	0.000000		
4	C	2.440968	2.710235	1.446759	0.000000	
5	H	3.413144	3.798657	2.166696	1.088792	0.000000
6	C	3.169563	3.029629	2.744842	2.054366	2.496700
7	H	4.055691	3.753157	3.486173	2.397735	2.530718
8	C	2.892669	2.362321	3.138121	2.867082	3.642991
9	H	3.548509	2.590854	3.980364	3.571045	4.377941
10	C	1.412791	2.528744	2.449723	3.742761	4.605344
11	H	2.167245	2.776338	3.433265	4.604724	5.546459
12	C	2.419104	3.775315	2.802490	4.244967	4.866377
13	H	3.404055	4.663857	3.888779	5.331055	5.937120
14	C	2.804581	4.251341	2.420659	3.767900	4.097800
15	H	3.890835	5.337563	3.406356	4.655577	4.805548
16	C	2.446994	3.739430	1.410421	2.516514	2.721880
17	H	3.429223	4.596720	2.162003	2.754907	2.509992
18	C	2.865595	2.439276	2.475207	1.448938	2.174702
19	C	2.499744	1.453861	2.862420	2.439245	3.415392
20	C	3.777633	2.531749	4.258544	3.740587	4.608991
21	H	4.127263	2.778772	4.897425	4.603216	5.549975
22	C	4.890352	3.781469	5.071659	4.247256	4.876608
23	H	5.852539	4.669188	6.127541	5.333527	5.948208
24	C	5.087365	4.257662	4.866328	3.771642	4.111006

This journal is © The Royal Society of Chemistry 2014

25	H	6.141637	5.344074	5.825830	4.659475	4.819745
26	C	4.258927	3.741697	3.743342	2.517923	2.733690
27	H	4.884887	4.599837	4.080067	2.757517	2.524014
28	C	3.081500	3.027861	3.477609	3.718100	4.431006
29	C	3.551106	3.916815	2.957757	2.774022	2.929183
30	O	3.387836	3.817506	3.281418	3.588136	4.014809
31	O	4.419725	4.961187	3.532253	3.292356	3.041542
32	O	3.659355	3.543046	4.362386	4.791287	5.571797
33	C	2.480003	1.435495	3.747293	4.139017	5.225597
34	N	3.537476	2.599125	4.867708	5.300023	6.385336
		6	7	8	9	10
6	C	0.000000				
7	H	1.083812	0.000000			
8	C	1.414673	2.206615	0.000000		
9	H	2.234128	2.660962	1.080987	0.000000	
10	C	4.326828	5.307639	3.895287	4.549121	0.000000
11	H	4.979626	5.967511	4.265013	4.728654	1.086009
12	C	4.982079	5.957446	4.833207	5.644845	1.384735
13	H	5.981539	6.985139	5.734202	6.509845	2.141044
14	C	4.729117	5.591673	4.986856	5.927406	2.428975
15	H	5.607406	6.429389	5.961590	6.938538	3.407245
16	C	3.707741	4.433856	4.256248	5.210168	2.816732
17	H	3.992385	4.525505	4.832367	5.807678	3.903123
18	C	2.654380	2.714313	3.067046	3.341352	4.262099
19	C	3.089245	3.406357	2.814160	2.804903	3.778609
20	C	4.209958	4.317510	3.778602	3.375338	4.912131
21	H	4.884237	5.108088	4.166045	3.615769	5.043270
22	C	4.832578	4.636065	4.693488	4.263638	6.114868
23	H	5.827778	5.590267	5.588675	5.022107	7.007040
24	C	4.570427	4.159320	4.850358	4.634107	6.424259
25	H	5.441636	4.883574	5.820470	5.571730	7.479544
26	C	3.570557	3.197663	4.147806	4.232452	5.639665
27	H	3.873795	3.339134	4.744797	4.960828	6.245405
28	C	2.332918	3.299514	1.474667	2.221609	3.583990
29	C	1.495028	2.216762	2.327721	3.331870	4.361095
30	O	2.334614	3.281975	2.330959	3.314067	3.819936
31	O	2.441898	2.805292	3.501630	4.470518	5.159782
32	O	3.511223	4.442510	2.438713	2.827305	3.791591
33	C	4.125772	4.860338	3.059961	2.935383	2.929442
34	N	5.140217	5.861369	3.933606	3.628173	3.673063
		11	12	13	14	15
11	H	0.000000				
12	C	2.150957	0.000000			
13	H	2.473853	1.086330	0.000000		
14	C	3.416476	1.410537	2.165378	0.000000	
15	H	4.306857	2.165865	2.488286	1.086315	0.000000
16	C	3.902599	2.425428	3.404593	1.385261	2.144499
17	H	4.988848	3.415065	4.307184	2.152804	2.480673
18	C	4.902317	5.069725	6.126506	4.862411	5.822219
19	C	4.131077	4.885728	5.849490	5.080553	6.135004
20	C	5.047353	6.109199	7.003455	6.416219	7.471782
21	H	4.941970	6.341748	7.128697	6.864912	7.937381

This journal is © The Royal Society of Chemistry 2014

22	C	6.351215	7.214293	8.156725	7.337933	8.348674
23	H	7.136423	8.154533	9.056198	8.352920	9.369373
24	C	6.875965	7.340421	8.357345	7.190514	8.123840
25	H	7.948533	8.350517	9.373186	8.122982	9.013199
26	C	6.265654	6.396514	7.455321	6.068595	6.954601
27	H	6.986979	6.821994	7.895922	6.275750	7.051230
28	C	3.868982	4.339761	5.072590	4.632208	5.509883
29	C	5.107678	4.655137	5.560742	4.228270	4.922547
30	O	4.385289	4.141585	4.887382	4.061151	4.766803
31	O	6.010260	5.181016	6.052475	4.458713	4.934471
32	O	3.762469	4.589955	5.114826	5.168612	6.010191
33	C	2.605424	4.312355	4.966242	5.142697	6.205707
34	N	3.029859	5.030599	5.500532	6.035276	7.061569

		16	17	18	19	20
16	C	0.000000				
17	H	1.086633	0.000000			
18	C	3.742941	4.080565	0.000000		
19	C	4.255715	4.881996	1.418390	0.000000	
20	C	5.635627	6.242410	2.445909	1.412191	0.000000
21	H	6.259681	6.982137	3.430086	2.167007	1.086259
22	C	6.397919	6.825271	2.802890	2.422008	1.386153
23	H	7.455501	7.898572	3.889256	3.406589	2.143012
24	C	6.072079	6.281535	2.422536	2.806934	2.428529
25	H	6.957369	7.056832	3.408266	3.893345	3.407919
26	C	4.857519	4.969179	1.409340	2.444740	2.812594
27	H	4.966902	4.837821	2.162058	3.427802	3.900054
28	C	4.244413	4.906743	4.268946	3.960618	4.999189
29	C	3.373380	3.537028	3.849112	4.327459	5.570282
30	O	3.634356	4.090724	4.557627	4.644942	5.866860
31	O	3.557051	3.366307	4.526104	5.254162	6.517532
32	O	5.057798	5.826678	5.230212	4.669426	5.557361
33	C	4.920983	5.870088	3.741587	2.472224	2.914226
34	N	5.970553	6.956925	4.846240	3.509035	3.616660

		21	22	23	24	25
21	H	0.000000				
22	C	2.150392	0.000000			
23	H	2.473188	1.086440	0.000000		
24	C	3.415259	1.410145	2.165714	0.000000	
25	H	4.306657	2.166286	2.489908	1.086507	0.000000
26	C	3.898829	2.424650	3.404964	1.386702	2.146863
27	H	4.986268	3.414464	4.307761	2.153071	2.481301
28	C	5.222213	6.053400	6.936634	6.259930	7.253097
29	C	6.184541	6.268863	7.285964	5.952323	6.801078
30	O	6.266155	6.800815	7.774821	6.743390	7.685958
31	O	7.222067	7.079912	8.117837	6.562507	7.309959
32	O	5.554755	6.728156	7.521259	7.128026	8.145714
33	C	2.588427	4.298406	4.949828	5.131515	6.194433
34	N	2.961386	4.970167	5.429770	5.985396	7.008568

		26	27	28	29	30
26	C	0.000000				
27	H	1.087497	0.000000			
28	C	5.476297	6.007159	0.000000		

29	C	4.820731	4.939225	2.281377	0.000000	
30	O	5.726032	6.026338	1.411157	1.385187	0.000000
31	O	5.321891	5.197454	3.423132	1.203006	2.269730
32	O	6.469542	7.088901	1.200924	3.410420	2.277195
33	C	4.910823	5.863201	3.426892	4.946235	4.526622
34	N	5.934457	6.927840	4.116367	5.913758	5.332817

	31	32	33	34	
31 O	0.000000				
32 O	4.484163	0.000000			
33 C	6.076778	3.463826	0.000000		
34 N	7.073996	3.832184	1.163776	0.000000	

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.531252	0.774422	0.983202
2	6	0	0.598888	1.172590	0.167051
3	6	0	-0.651280	-0.615631	1.251234
4	6	0	0.331499	-1.482859	0.638720
5	1	0	0.207771	-2.552659	0.798990
6	6	0	-0.159133	-1.337374	-1.350888
7	1	0	0.541784	-2.100576	-1.668516
8	6	0	-0.089049	0.011422	-1.771762
9	1	0	0.717556	0.472256	-2.324530
10	6	0	-1.523790	1.664779	1.450223
11	1	0	-1.444715	2.724604	1.226763
12	6	0	-2.581987	1.180248	2.200516
13	1	0	-3.333346	1.869032	2.576215
14	6	0	-2.699619	-0.198911	2.471989
15	1	0	-3.540399	-0.563962	3.055004
16	6	0	-1.757930	-1.090727	1.985331
17	1	0	-1.858995	-2.157242	2.167268
18	6	0	1.686119	-0.981654	0.523744
19	6	0	1.829346	0.402616	0.249680
20	6	0	3.114381	0.935372	0.006492
21	1	0	3.226467	1.993602	-0.211555
22	6	0	4.226988	0.111030	0.069633
23	1	0	5.216277	0.529616	-0.092988
24	6	0	4.085214	-1.265089	0.342953
25	1	0	4.965609	-1.900036	0.390330
26	6	0	2.826585	-1.809247	0.549560
27	1	0	2.711042	-2.871847	0.750012
28	6	0	-1.470157	0.500528	-1.938970
29	6	0	-1.610936	-1.693689	-1.330467
30	8	0	-2.343684	-0.540623	-1.559076

```
   31          8             0       -2.131877   -2.759991   -1.133376
   32          8             0       -1.893279    1.557238   -2.321789
   33          6             0        0.697475    2.544077   -0.245197
   34          7             0        0.801926    3.653259   -0.581618
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3915430      0.2665331
0.2437751
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1864.4899018576 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A)

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB+HF-LYP) = -1011.05929350 A.U. after 15 cycles
Convg = 0.5773D-08 -V/T = 2.0094
S**2 = 0.0000
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000022060	0.000056259	0.000014862
2	6	-0.000037412	-0.000141110	-0.000299375
3	6	-0.000082732	0.000026463	-0.000040057
4	6	0.000041453	-0.000065959	0.000059854
5	1	-0.000000217	-0.000038653	0.000014507
6	6	-0.000086638	-0.000026240	0.000080632
7	1	0.000027653	0.000025356	0.000016186
8	6	0.000044820	0.000120403	-0.000102499
9	1	0.000006209	-0.000004380	0.000000234
10	6	0.000018331	-0.000005682	0.000006890
11	1	-0.000001288	-0.000003482	0.000003506
12	6	-0.000014019	0.000007735	0.000015088
13	1	-0.000001677	-0.000002908	0.000002215
14	6	-0.000011622	0.000007386	-0.000014527
15	1	-0.000001159	-0.000003346	0.000002953
16	6	0.000014825	-0.000019013	-0.000009443
17	1	0.000001827	0.000001000	0.000003180
18	6	0.000053972	0.000015141	-0.000008585
19	6	0.000045772	0.000017743	0.000002051
20	6	-0.000007764	0.000006001	-0.000009166
21	1	-0.000000056	0.000000878	0.000000489
22	6	0.000012961	0.000003690	0.000003972
23	1	-0.000000741	0.000003679	-0.000001505
24	6	0.000003161	0.000001336	-0.000007401
25	1	0.000000636	0.000002699	-0.000001807
26	6	-0.000011948	-0.000000167	-0.000000603
27	1	0.000000466	0.000002656	-0.000001728
28	6	-0.000012752	-0.000041364	-0.000002030
29	6	0.000003697	-0.000017587	-0.000001765

```
   30          8           0.000006406    0.000002323    0.000021462
   31          8          -0.000008148    0.000004328    0.000011496
   32          8          -0.000008331   -0.000006866   -0.000001216
   33          6           0.000016295    0.000051321    0.000217208
   34          7           0.000010076    0.000020359    0.000024922
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000299375 RMS     0.000048640


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000241046 RMS     0.000026269
 Search for a saddle point.
 Step number   5 out of a maximum of 195
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Swaping is turned off.
 Update second derivatives using D2CorX and points  3  4  5
     Eigenvalues ---   -0.02408   0.00225   0.00735   0.00807
0.01153
     Eigenvalues ---    0.01222   0.01485   0.01550   0.01608
0.01646
     Eigenvalues ---    0.01762   0.01809   0.01905   0.01920
0.01949
     Eigenvalues ---    0.02015   0.02113   0.02168   0.02222
0.02271
     Eigenvalues ---    0.02404   0.02475   0.02493   0.02514
0.02714
     Eigenvalues ---    0.02759   0.02770   0.02778   0.03434
0.04002
     Eigenvalues ---    0.05468   0.06598   0.06982   0.07494
0.08509
     Eigenvalues ---    0.10376   0.11081   0.11156   0.11193
0.11822
     Eigenvalues ---    0.11898   0.12501   0.12521   0.12651
0.12704
     Eigenvalues ---    0.12924   0.14218   0.16407   0.17464
0.18047
     Eigenvalues ---    0.19144   0.19172   0.19200   0.19397
0.19562
     Eigenvalues ---    0.19760   0.20284   0.20983   0.23494
0.23970
     Eigenvalues ---    0.25107   0.25140   0.26075   0.27928
0.28526
     Eigenvalues ---    0.29525   0.30083   0.30948   0.31757
0.33457
     Eigenvalues ---    0.34193   0.35306   0.35873   0.35904
0.36040
     Eigenvalues ---    0.36126   0.36225   0.36265   0.36292
0.36350
     Eigenvalues ---    0.37230   0.38018   0.39098   0.40149
0.40788
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.41730   0.42416   0.42886   0.44734
0.47342
     Eigenvalues ---    0.47621   0.50294   0.50636   0.88539
0.89747
     Eigenvalues ---
1.375131000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
          1            -0.05185   0.02418   0.15344   0.01857
0.40685
                           R6        R7        R8        R9        R10
          1             0.14384  -0.05407  -0.03954  -0.05544
0.16955
                           R11       R12       R13       R14       R15
          1             0.01903  -0.00645   0.42284   0.16232  -
0.05533
                           R16       R17       R18       R19       R20
```

This journal is © The Royal Society of Chemistry 2014

1	0.28400	-0.00647	-0.09553	0.17873	-0.01030

	R21	R22	R23	R24	R25
1	-0.02192	-0.00913	0.14726	-0.00903	-0.06241

	R26	R27	R28	R29	R30
1	0.05596	-0.00028	-0.01457	0.00002	0.01604

	R31	R32	R33	R34	R35
1	-0.00011	-0.01546	-0.00020	0.02059	0.01825

	R36	R37	R38	R39	R40
1	0.01830	-0.00006	-0.01410	0.00006	0.01545

	R41	R42	R43	R44	R45
1	-0.00006	-0.01494	-0.00008	0.00188	0.00206

	R46	R47	R48	A1	A2
1	-0.00195	0.00210	-0.00067	0.02196	-0.01168

	A3	A4	A5	A6	A7
1	-0.00964	0.04533	0.01870	0.01691	0.01898

	A8	A9	A10	A11	A12
1	-0.00481	-0.01324	0.03080	0.05548	0.02809

	A13	A14	A15	A16	A17
1	0.06015	0.03817	0.02025	0.04584	0.00956

	A18	A19	A20	A21	A22
1	0.02076	-0.00621	0.00607	0.00013	0.00067

	A23	A24	A25	A26	A27
1	0.00281	-0.00347	-0.00241	0.00095	0.00147

	A28	A29	A30	A31	A32
1	0.00470	-0.00599	0.00128	0.01916	-0.01407

	A33	A34	A35	A36	A37
1	-0.00420	0.02355	-0.01351	-0.00947	-0.00628

	A38	A39	A40	A41	A42
1	0.00623	0.00001	0.00106	0.00225	-0.00331

	A43	A44	A45	A46	A47
1	-0.00230	0.00049	0.00181	0.00474	-0.00584

	A48	A49	A50	A51	A52
1	0.00104	-0.00205	0.00284	-0.00079	-0.00632

	A53	A54	A55	A56	A57

This journal is © The Royal Society of Chemistry 2014

```
          1              0.00374   0.00270  -0.01380  -0.00336
0.01558
                           D1        D2        D3        D4        D5
          1              0.16608  -0.03373   0.15359  -0.04621  -
0.00032
                           D6        D7        D8        D9        D10
          1             -0.01025   0.01144   0.00152   0.01075
0.01154
                           D11       D12       D13       D14       D15
          1             -0.00313  -0.00234  -0.16522  -0.15448
0.03323
                           D16       D17       D18       D19       D20
          1              0.04396   0.04646  -0.16071   0.05739  -
0.14977
                           D21       D22       D23       D24       D25
          1              0.00037   0.00257  -0.01211  -0.00991
0.16099
                           D26       D27       D28       D29       D30
          1              0.15107  -0.04826  -0.05818  -0.00138
0.16901
                           D31       D32       D33       D34       D35
          1             -0.17222  -0.00184  -0.14175  -0.14809
0.02800
                           D36       D37       D38       D39       D40
          1              0.02166  -0.02411  -0.02322   0.14135
0.14225
                           D41       D42       D43       D44       D45
          1              0.00046   0.00111   0.00130   0.00195  -
0.00087
                           D46       D47       D48       D49       D50
          1              0.00054  -0.00020   0.00121  -0.00127  -
0.00352
                           D51       D52       D53       D54       D55
          1              0.00012  -0.00213  -0.00115  -0.01115
0.00768
                           D56       D57       D58       D59       D60
          1             -0.00232   0.01229   0.00881   0.00080  -
0.00267
                           D61       D62       D63       D64       D65
          1             -0.00793  -0.00983   0.00420   0.00230
0.00083
                           D66       D67       D68       D69       D70
          1             -0.00058  -0.00116  -0.00257   0.00132  -
0.00080
                           D71       D72       D73       D74       D75
          1             -0.00009  -0.00221   0.00066   0.00425  -
0.00146
                           D76       D77       D78       D79       D80
          1              0.00213   0.04422   0.04345  -0.04716  -
0.04132
 RFO step:  Lambda0=7.722967241D-08 Lambda=-7.67588030D-07.
 Linear search not attempted -- option 19 set.
```

This journal is © The Royal Society of Chemistry 2014

```
 Iteration  1 RMS(Cart)=  0.00067999 RMS(Int)=  0.00000024
 Iteration  2 RMS(Cart)=  0.00000027 RMS(Int)=  0.00000006
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.73968   0.00004   0.00000   0.00013   0.00013
2.73981
    R2        2.68480   0.00001   0.00000   0.00002   0.00002
2.68483
    R3        5.46635   0.00000   0.00000   0.00084   0.00084
5.46719
    R4        2.66979  -0.00001   0.00000  -0.00001  -0.00001
2.66977
    R5        4.46414   0.00004   0.00000   0.00132   0.00132
4.46547
    R6        4.89600  -0.00004   0.00000   0.00096   0.00096
4.89697
    R7        2.74740   0.00004   0.00000   0.00013   0.00013
2.74753
    R8        2.71269  -0.00024   0.00000  -0.00107  -0.00107
2.71162
    R9        2.73398   0.00009   0.00000   0.00021   0.00021
2.73419
   R10        5.18700   0.00003   0.00000  -0.00003  -0.00003
5.18697
   R11        2.66531  -0.00001   0.00000  -0.00003  -0.00003
2.66528
   R12        2.05752   0.00004   0.00000   0.00005   0.00005
2.05757
   R13        3.88219  -0.00003   0.00000   0.00052   0.00052
3.88271
   R14        4.53106  -0.00004   0.00000  -0.00150  -0.00150
4.52957
   R15        2.73810   0.00004   0.00000   0.00006   0.00006
2.73816
   R16        4.71808  -0.00004   0.00000  -0.00035  -0.00035
4.71773
   R17        2.04811   0.00004   0.00000   0.00004   0.00004
2.04815
   R18        2.67334   0.00008   0.00000   0.00005   0.00005
2.67339
   R19        5.01605   0.00005   0.00000   0.00108   0.00108
5.01713
   R20        2.82519  -0.00001   0.00000  -0.00006  -0.00006
2.82513
   R21        5.12931  -0.00001   0.00000  -0.00047  -0.00047
5.12884
   R22        2.04277   0.00003   0.00000   0.00000   0.00000
2.04276
   R23        5.31799   0.00004   0.00000   0.00051   0.00051
5.31850
```

This journal is © The Royal Society of Chemistry 2014

R24	2.78672	0.00003	0.00000	0.00003	0.00003
2.78675					
R25	5.30050	-0.00002	0.00000	-0.00027	-0.00027
5.30023					
R26	5.54707	-0.00001	0.00000	0.00302	0.00301
5.55008					
R27	2.05226	0.00000	0.00000	0.00000	0.00000
2.05226					
R28	2.61677	0.00001	0.00000	0.00001	0.00001
2.61678					
R29	2.05287	0.00000	0.00000	0.00000	0.00000
2.05286					
R30	2.66553	-0.00001	0.00000	-0.00003	-0.00003
2.66550					
R31	2.05284	0.00000	0.00000	0.00000	0.00000
2.05284					
R32	2.61776	0.00002	0.00000	0.00003	0.00003
2.61780					
R33	2.05344	0.00000	0.00000	0.00000	0.00000
2.05344					
R34	2.68037	0.00002	0.00000	0.00008	0.00008
2.68045					
R35	2.66327	-0.00001	0.00000	0.00001	0.00001
2.66327					
R36	2.66865	0.00000	0.00000	0.00003	0.00003
2.66868					
R37	2.05273	0.00000	0.00000	0.00000	0.00000
2.05273					
R38	2.61945	0.00001	0.00000	0.00000	0.00000
2.61945					
R39	2.05307	0.00000	0.00000	0.00000	0.00000
2.05307					
R40	2.66479	0.00000	0.00000	0.00001	0.00001
2.66480					
R41	2.05320	0.00000	0.00000	0.00000	0.00000
2.05320					
R42	2.62049	0.00001	0.00000	0.00000	0.00000
2.62049					
R43	2.05507	0.00000	0.00000	0.00000	0.00000
2.05507					
R44	2.66670	0.00002	0.00000	0.00013	0.00013
2.66683					
R45	2.26942	0.00000	0.00000	0.00000	0.00000
2.26942					
R46	2.61762	-0.00001	0.00000	-0.00009	-0.00009
2.61754					
R47	2.27335	0.00002	0.00000	0.00003	0.00003
2.27338					
R48	2.19922	-0.00003	0.00000	-0.00001	-0.00001
2.19921					
A1	2.02725	0.00001	0.00000	0.00016	0.00016
2.02742					

This journal is © The Royal Society of Chemistry 2014

A2	2.16597	-0.00002	0.00000	-0.00014	-0.00014
2.16583					
A3	2.08850	0.00001	0.00000	-0.00002	-0.00002
2.08847					
A4	2.07407	-0.00002	0.00000	-0.00012	-0.00012
2.07396					
A5	2.06872	0.00001	0.00000	-0.00005	-0.00005
2.06866					
A6	2.05351	-0.00001	0.00000	-0.00004	-0.00004
2.05348					
A7	2.03669	0.00001	0.00000	0.00004	0.00004
2.03673					
A8	2.08754	-0.00001	0.00000	-0.00003	-0.00003
2.08751					
A9	2.15488	0.00000	0.00000	0.00001	0.00001
2.15488					
A10	2.03696	0.00002	0.00000	0.00022	0.00022
2.03717					
A11	2.05028	-0.00003	0.00000	-0.00001	-0.00001
2.05027					
A12	2.04631	0.00001	0.00000	0.00010	0.00010
2.04641					
A13	2.15575	0.00000	0.00000	0.00027	0.00026
2.15602					
A14	2.05351	-0.00002	0.00000	0.00029	0.00029
2.05381					
A15	1.85397	0.00003	0.00000	0.00020	0.00020
1.85417					
A16	2.20875	0.00001	0.00000	-0.00005	-0.00005
2.20870					
A17	1.87923	-0.00005	0.00000	-0.00016	-0.00016
1.87907					
A18	2.09377	0.00001	0.00000	0.00006	0.00006
2.09383					
A19	2.08960	-0.00001	0.00000	-0.00004	-0.00004
2.08957					
A20	2.08917	0.00001	0.00000	0.00006	0.00006
2.08923					
A21	2.10436	0.00000	0.00000	-0.00002	-0.00002
2.10433					
A22	2.08757	0.00000	0.00000	0.00000	0.00000
2.08758					
A23	2.10614	-0.00001	0.00000	-0.00005	-0.00005
2.10609					
A24	2.08944	0.00001	0.00000	0.00004	0.00004
2.08948					
A25	2.09025	0.00000	0.00000	0.00002	0.00002
2.09027					
A26	2.10037	0.00000	0.00000	-0.00001	-0.00001
2.10036					
A27	2.09249	0.00000	0.00000	-0.00001	-0.00001
2.09247					

This journal is © The Royal Society of Chemistry 2014

A28	2.09367	0.00001	0.00000	0.00004	0.00004
2.09371					
A29	2.08373	0.00000	0.00000	0.00000	0.00000
2.08372					
A30	2.10578	0.00000	0.00000	-0.00004	-0.00004
2.10574					
A31	2.03457	0.00001	0.00000	0.00008	0.00008
2.03465					
A32	2.15551	0.00000	0.00000	-0.00005	-0.00005
2.15546					
A33	2.08854	-0.00001	0.00000	-0.00003	-0.00003
2.08851					
A34	2.02905	0.00002	0.00000	0.00013	0.00013
2.02918					
A35	2.16584	-0.00002	0.00000	-0.00011	-0.00011
2.16573					
A36	2.08672	0.00000	0.00000	-0.00001	-0.00001
2.08671					
A37	2.08976	0.00000	0.00000	0.00000	0.00000
2.08976					
A38	2.09231	0.00000	0.00000	0.00002	0.00002
2.09232					
A39	2.10096	0.00000	0.00000	-0.00002	-0.00002
2.10094					
A40	2.08856	0.00000	0.00000	0.00000	0.00000
2.08856					
A41	2.10421	0.00000	0.00000	-0.00001	-0.00001
2.10420					
A42	2.09041	0.00000	0.00000	0.00001	0.00001
2.09042					
A43	2.09125	0.00000	0.00000	-0.00001	-0.00001
2.09124					
A44	2.09795	0.00000	0.00000	0.00001	0.00001
2.09796					
A45	2.09398	0.00000	0.00000	0.00000	0.00000
2.09398					
A46	2.09592	0.00000	0.00000	0.00002	0.00002
2.09594					
A47	2.08424	0.00000	0.00000	-0.00001	-0.00001
2.08423					
A48	2.10287	0.00000	0.00000	-0.00002	-0.00002
2.10286					
A49	1.88022	0.00001	0.00000	0.00002	0.00002
1.88024					
A50	2.28891	0.00001	0.00000	0.00004	0.00004
2.28895					
A51	2.11404	-0.00001	0.00000	-0.00006	-0.00006
2.11398					
A52	1.88919	-0.00001	0.00000	-0.00006	-0.00006
1.88914					
A53	2.25751	0.00001	0.00000	0.00002	0.00002
2.25753					

This journal is © The Royal Society of Chemistry 2014

A54	2.13625	0.00000	0.00000	0.00004	0.00004	2.13629
A55	1.90831	0.00002	0.00000	0.00004	0.00004	1.90835
A56	3.16084	0.00000	0.00000	-0.00009	-0.00009	3.16075
A57	3.12358	-0.00002	0.00000	-0.00094	-0.00094	3.12264
D1	-0.55094	-0.00001	0.00000	0.00018	0.00018	-0.55077
D2	3.03611	0.00005	0.00000	0.00069	0.00069	3.03680
D3	2.64906	-0.00001	0.00000	0.00021	0.00021	2.64927
D4	-0.04707	0.00005	0.00000	0.00072	0.00072	-0.04635
D5	-0.04212	0.00001	0.00000	0.00018	0.00018	-0.04194
D6	-3.09014	0.00000	0.00000	-0.00009	-0.00009	-3.09023
D7	3.04381	0.00002	0.00000	0.00015	0.00015	3.04396
D8	-0.00421	0.00000	0.00000	-0.00012	-0.00012	-0.00433
D9	-0.03636	0.00001	0.00000	0.00012	0.00012	-0.03624
D10	3.11658	0.00000	0.00000	0.00007	0.00007	3.11666
D11	-3.11761	0.00000	0.00000	0.00014	0.00014	-3.11747
D12	0.03533	0.00000	0.00000	0.00009	0.00009	0.03542
D13	0.55214	0.00000	0.00000	-0.00032	-0.00032	0.55182
D14	-2.65001	0.00001	0.00000	-0.00028	-0.00028	-2.65029
D15	-3.03106	-0.00005	0.00000	-0.00083	-0.00083	-3.03189
D16	0.04998	-0.00004	0.00000	-0.00079	-0.00080	0.04918
D17	-3.08466	-0.00001	0.00000	0.00019	0.00019	-3.08447
D18	0.63186	-0.00002	0.00000	-0.00037	-0.00037	0.63149
D19	-0.04061	0.00000	0.00000	0.00047	0.00047	-0.04014
D20	-2.60727	0.00000	0.00000	-0.00009	-0.00009	-2.60736
D21	-0.03148	0.00000	0.00000	0.00005	0.00005	-0.03143
D22	3.11544	0.00001	0.00000	0.00022	0.00022	3.11566

This journal is © The Royal Society of Chemistry 2014

D23	-3.07284	-0.00002	0.00000	-0.00024	-0.00024	-3.07307
D24	0.07408	-0.00001	0.00000	-0.00007	-0.00007	0.07402
D25	-0.63044	0.00002	0.00000	0.00022	0.00022	-0.63022
D26	2.61420	0.00001	0.00000	0.00021	0.00021	2.61441
D27	3.08918	0.00000	0.00000	-0.00038	-0.00038	3.08880
D28	0.05064	0.00000	0.00000	-0.00039	-0.00039	0.05024
D29	-0.16122	0.00004	0.00000	0.00072	0.00072	-0.16050
D30	2.50416	-0.00003	0.00000	0.00042	0.00042	2.50458
D31	-2.61490	0.00004	0.00000	-0.00040	-0.00040	-2.61530
D32	0.05048	-0.00003	0.00000	-0.00070	-0.00070	0.04978
D33	-2.63266	0.00001	0.00000	-0.00042	-0.00042	-2.63308
D34	0.53173	0.00001	0.00000	-0.00035	-0.00035	0.53138
D35	-0.13163	0.00002	0.00000	0.00061	0.00061	-0.13103
D36	3.03275	0.00001	0.00000	0.00068	0.00068	3.03343
D37	0.04511	0.00003	0.00000	0.00056	0.00056	0.04568
D38	-3.09078	0.00003	0.00000	0.00062	0.00062	-3.09016
D39	2.74767	-0.00003	0.00000	0.00025	0.00025	2.74792
D40	-0.38822	-0.00003	0.00000	0.00031	0.00031	-0.38792
D41	3.11964	0.00000	0.00000	0.00001	0.00001	3.11965
D42	-0.03121	0.00000	0.00000	0.00000	0.00000	-0.03121
D43	-0.01051	0.00000	0.00000	-0.00004	-0.00004	-0.01054
D44	3.12183	0.00000	0.00000	-0.00005	-0.00005	3.12178
D45	-3.13248	0.00000	0.00000	-0.00009	-0.00009	-3.13257
D46	-0.00469	0.00000	0.00000	-0.00007	-0.00007	-0.00476
D47	-0.00015	0.00000	0.00000	-0.00010	-0.00010	-0.00025
D48	3.12764	0.00000	0.00000	-0.00008	-0.00008	3.12755

This journal is © The Royal Society of Chemistry 2014

D49	0.03618	0.00000	0.00000	0.00004	0.00004	0.03622
D50	-3.11081	-0.00001	0.00000	-0.00013	-0.00013	-3.11094
D51	-3.11924	0.00000	0.00000	0.00006	0.00006	-3.11917
D52	0.01696	0.00000	0.00000	-0.00011	-0.00011	0.01685
D53	0.04063	0.00000	0.00000	0.00010	0.00010	0.04073
D54	-3.04331	-0.00001	0.00000	0.00007	0.00007	-3.04325
D55	3.08335	0.00001	0.00000	0.00011	0.00011	3.08345
D56	-0.00060	0.00000	0.00000	0.00007	0.00007	-0.00053
D57	3.06523	0.00001	0.00000	0.00000	0.00000	3.06523
D58	-0.09519	0.00000	0.00000	-0.00012	-0.00012	-0.09531
D59	0.02972	0.00000	0.00000	-0.00002	-0.00002	0.02970
D60	-3.13070	0.00000	0.00000	-0.00014	-0.00014	-3.13084
D61	0.05390	-0.00001	0.00000	-0.00017	-0.00017	0.05373
D62	-3.10685	-0.00001	0.00000	-0.00011	-0.00011	-3.10696
D63	3.13305	0.00000	0.00000	-0.00012	-0.00012	3.13293
D64	-0.02770	0.00000	0.00000	-0.00006	-0.00006	-0.02776
D65	-3.11437	0.00000	0.00000	-0.00002	-0.00002	-3.11440
D66	0.02723	0.00000	0.00000	0.00000	0.00000	0.02723
D67	0.00794	0.00000	0.00000	0.00003	0.00003	0.00797
D68	-3.13364	0.00000	0.00000	0.00006	0.00006	-3.13359
D69	-3.14086	0.00000	0.00000	0.00007	0.00007	-3.14079
D70	0.00203	0.00000	0.00000	0.00006	0.00006	0.00209
D71	0.00075	0.00000	0.00000	0.00009	0.00009	0.00084
D72	-3.13956	0.00000	0.00000	0.00008	0.00008	-3.13947
D73	-0.03063	0.00000	0.00000	-0.00005	-0.00005	-0.03067
D74	3.13000	0.00000	0.00000	0.00007	0.00007	3.13007

```
   D75        3.11226   0.00000   0.00000  -0.00006  -0.00006
3.11220
   D76       -0.01030   0.00000   0.00000   0.00006   0.00006  -
0.01024
   D77       -0.13100  -0.00002   0.00000  -0.00017  -0.00017  -
0.13117
   D78        3.00558  -0.00002   0.00000  -0.00022  -0.00022
3.00536
   D79        0.16285   0.00000   0.00000  -0.00027  -0.00027
0.16257
   D80       -2.99962   0.00000   0.00000  -0.00034  -0.00034  -
2.99996
         Item               Value     Threshold  Converged?
 Maximum Force            0.000241     0.000450     YES
 RMS     Force            0.000026     0.000300     YES
 Maximum Displacement     0.005019     0.001800     NO
 RMS     Displacement     0.000680     0.001200     YES
 Predicted change in Energy=-3.451819D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.559656    1.134053   -0.760894
    2          6             0        0.534139    0.448118   -1.420563
    3          6             0       -0.563909    1.085797    0.659030
    4          6             0        0.488312    0.315954    1.286416
    5          1             0        0.453901    0.233081    2.371530
    6          6             0       -0.011765   -1.601589    0.743735
    7          1             0        0.750622   -2.065494    1.358755
    8          6             0       -0.053157   -1.712798   -0.665979
    9          1             0        0.713200   -2.134296   -1.301246
   10          6             0       -1.623233    1.767069   -1.442108
   11          1             0       -1.632427    1.784872   -2.527931
   12          6             0       -2.638118    2.371198   -0.719234
   13          1             0       -3.444487    2.875245   -1.244416
   14          6             0       -2.640820    2.328847    0.690651
   15          1             0       -3.448755    2.800511    1.242787
   16          6             0       -1.627809    1.675303    1.373063
   17          1             0       -1.639909    1.615181    2.457965
   18          6             0        1.796586    0.340647    0.664062
   19          6             0        1.824317    0.382063   -0.753493
   20          6             0        3.060755    0.287283   -1.429188
   21          1             0        3.084545    0.310556   -2.514935
   22          6             0        4.238071    0.188075   -0.704268
   23          1             0        5.189204    0.140938   -1.227216
   24          6             0        4.211109    0.147845    0.705050
   25          1             0        5.141266    0.070715    1.261246
```

26	6	0	3.001979	0.204872	1.381586
27	1	0	2.975156	0.163421	2.467959
28	6	0	-1.469900	-1.795264	-1.066895
29	6	0	-1.429005	-1.688146	1.211651
30	8	0	-2.254536	-1.671278	0.099524
31	8	0	-1.859942	-1.740754	2.333608
32	8	0	-1.978830	-1.944199	-2.144408
33	6	0	0.518877	0.352191	-2.852201
34	7	0	0.531357	0.272627	-4.013184

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.449847	0.000000			
3	C	1.420749	2.436606	0.000000		
4	C	2.441106	2.710591	1.446873	0.000000	
5	H	3.413375	3.799032	2.166961	1.088818	0.000000
6	C	3.169831	3.030428	2.744828	2.054642	2.496513
7	H	4.055471	3.753628	3.485433	2.396943	2.529270
8	C	2.893115	2.363022	3.138256	2.867207	3.642803
9	H	3.548838	2.591363	3.980287	3.570756	4.377328
10	C	1.412784	2.528705	2.449710	3.742887	4.605588
11	H	2.167216	2.776181	3.433243	4.604834	5.546669
12	C	2.419146	3.775356	2.802537	4.245142	4.866719
13	H	3.404085	4.663844	3.888825	5.331228	5.937468
14	C	2.804596	4.251439	2.420689	3.768043	4.098157
15	H	3.890849	5.337661	3.406369	4.655687	4.805880
16	C	2.446972	3.739565	1.410406	2.516606	2.722215
17	H	3.429210	4.596900	2.161988	2.754966	2.510321
18	C	2.865636	2.439464	2.475320	1.448970	2.174815
19	C	2.499775	1.453928	2.862532	2.439367	3.415554
20	C	3.777699	2.531744	4.258693	3.740694	4.609130
21	H	4.127349	2.778695	4.897578	4.603338	5.550120
22	C	4.890426	3.781509	5.071834	4.247336	4.876731
23	H	5.852618	4.669195	6.127724	5.333607	5.948324
24	C	5.087415	4.257758	4.866484	3.771666	4.111087
25	H	6.141681	5.344170	5.825983	4.659480	4.819801
26	C	4.258972	3.741850	3.743485	2.517920	2.733768
27	H	4.884927	4.600024	4.080194	2.757481	2.524060
28	C	3.082707	3.028864	3.478527	3.718860	4.431475
29	C	3.551268	3.917410	2.957793	2.774547	2.929466
30	O	3.388631	3.818274	3.282183	3.589015	4.015499
31	O	4.419411	4.961510	3.531756	3.292561	3.041601
32	O	3.661121	3.544312	4.363730	4.792248	5.572470
33	C	2.479538	1.434929	3.746911	4.138888	5.225493
34	N	3.536913	2.598555	4.867282	5.299952	6.385306

		6	7	8	9	10
6	C	0.000000				
7	H	1.083832	0.000000			
8	C	1.414699	2.206808	0.000000		
9	H	2.234121	2.661154	1.080985	0.000000	
10	C	4.326961	5.307407	3.895766	4.549661	0.000000

This journal is © The Royal Society of Chemistry 2014

11	H	4.979805	5.967460	4.265520	4.729334	1.086008
12	C	4.982073	5.957000	4.833621	5.645312	1.384742
13	H	5.981502	6.984723	5.734619	6.510384	2.141052
14	C	4.728962	5.590929	4.987118	5.927626	2.428938
15	H	5.607177	6.428547	5.961831	6.938753	3.407226
16	C	3.707516	4.432912	4.256343	5.210115	2.816671
17	H	3.992123	4.524408	4.832417	5.807527	3.903065
18	C	2.654950	2.714066	3.067115	3.340884	4.262135
19	C	3.089945	3.406604	2.814429	2.804760	3.778629
20	C	4.210678	4.317974	3.778791	3.375119	4.912197
21	H	4.884911	5.108648	4.166266	3.615746	5.043368
22	C	4.833292	4.636479	4.693551	4.263156	6.114942
23	H	5.828475	5.590760	5.588710	5.021632	7.007124
24	C	4.571070	4.159468	4.850327	4.633439	6.424307
25	H	5.442256	4.883713	5.820408	5.571015	7.479585
26	C	3.571107	3.197451	4.147751	4.231761	5.639707
27	H	3.874262	3.338704	4.744728	4.960126	6.245438
28	C	2.332820	3.299625	1.474685	2.221663	3.585319
29	C	1.494994	2.216936	2.327887	3.332078	4.361040
30	O	2.334499	3.282080	2.331049	3.314212	3.820655
31	O	2.441889	2.805502	3.501825	4.470805	5.159155
32	O	3.511139	4.442609	2.438753	2.827381	3.793835
33	C	4.126692	4.861179	3.061204	2.936978	2.928972
34	N	5.141589	5.862816	3.935397	3.630558	3.672335

		11	12	13	14	15
11	H	0.000000				
12	C	2.150948	0.000000			
13	H	2.473841	1.086329	0.000000		
14	C	3.416436	1.410524	2.165390	0.000000	
15	H	4.306842	2.165864	2.488329	1.086314	0.000000
16	C	3.902536	2.425429	3.404612	1.385279	2.144506
17	H	4.988788	3.415052	4.307190	2.152799	2.480643
18	C	4.902319	5.069837	6.126608	4.862532	5.822323
19	C	4.131051	4.885812	5.849552	5.080647	6.135089
20	C	5.047372	6.109328	7.003560	6.416359	7.471913
21	H	4.942024	6.341897	7.128822	6.865063	7.937528
22	C	6.351240	7.214446	8.156859	7.338110	8.348840
23	H	7.136458	8.154697	9.056344	8.353110	9.369556
24	C	6.875968	7.340558	8.357468	7.190682	8.123996
25	H	7.948529	8.350649	9.373307	8.123153	9.013356
26	C	6.265656	6.396649	7.455448	6.068760	6.954752
27	H	6.986976	6.822120	7.896046	6.275913	7.051377
28	C	3.870196	4.341084	5.073871	4.633392	5.511048
29	C	5.107613	4.654949	5.560483	4.228023	4.922235
30	O	4.385831	4.142357	4.888050	4.061976	4.767610
31	O	6.009689	5.180111	6.051486	4.457660	4.933285
32	O	3.764712	4.592215	5.117146	5.170562	6.012158
33	C	2.604963	4.311908	4.965785	5.142242	6.205263
34	N	3.028997	5.029879	5.499730	6.034634	7.060929

		16	17	18	19	20
16	C	0.000000				
17	H	1.086633	0.000000			

This journal is © The Royal Society of Chemistry 2014

18	C	3.743056	4.080688	0.000000		
19	C	4.255807	4.882100	1.418431	0.000000	
20	C	5.635765	6.242556	2.445949	1.412206	0.000000
21	H	6.259820	6.982280	3.430126	2.167017	1.086257
22	C	6.398101	6.825467	2.802937	2.422036	1.386155
23	H	7.455696	7.898781	3.889303	3.406614	2.143014
24	C	6.072259	6.281735	2.422555	2.806952	2.428524
25	H	6.957556	7.057042	3.408281	3.893361	3.407912
26	C	4.857693	4.969375	1.409343	2.444759	2.812596
27	H	4.967079	4.838030	2.162055	3.427825	3.900054
28	C	4.245371	4.907614	4.269457	3.961167	4.999509
29	C	3.373184	3.536912	3.849713	4.328008	5.570843
30	O	3.635148	4.091555	4.558304	4.645524	5.867303
31	O	3.556118	3.365439	4.526567	5.254551	6.518039
32	O	5.059310	5.828026	5.230850	4.670125	5.557739
33	C	4.920543	5.869698	3.741227	2.471769	2.913816
34	N	5.970021	6.956480	4.845829	3.508462	3.615951

		21	22	23	24	25
21	H	0.000000				
22	C	2.150381	0.000000			
23	H	2.473172	1.086440	0.000000		
24	C	3.415248	1.410149	2.165726	0.000000	
25	H	4.306642	2.166283	2.489914	1.086506	0.000000
26	C	3.898828	2.424663	3.404980	1.386704	2.146864
27	H	4.986266	3.414467	4.307764	2.153061	2.481287
28	C	5.222477	6.053599	6.936732	6.260138	7.253250
29	C	6.185012	6.269505	7.286584	5.953015	6.801802
30	O	6.266486	6.801266	7.775194	6.743919	7.686484
31	O	7.222478	7.080596	8.118540	6.563282	7.310834
32	O	5.555086	6.728332	7.521286	7.128211	8.145804
33	C	2.588075	4.298017	4.949461	5.131117	6.194042
34	N	2.960567	4.969486	5.429042	5.984803	7.007969

		26	27	28	29	30
26	C	0.000000				
27	H	1.087495	0.000000			
28	C	5.476615	6.007509	0.000000		
29	C	4.821412	4.939964	2.281429	0.000000	
30	O	5.726655	6.027046	1.411226	1.385140	0.000000
31	O	5.322602	5.198279	3.423233	1.203022	2.269727
32	O	6.469899	7.089285	1.200926	3.410425	2.277220
33	C	4.910443	5.862852	3.428427	4.946929	4.527574
34	N	5.933978	6.927430	4.118473	5.914942	5.334260

		31	32	33	34
31	O	0.000000			
32	O	4.484211	0.000000		
33	C	6.077155	3.465966	0.000000	
34	N	7.074869	3.835059	1.163773	0.000000

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96
Full point group C1
Largest Abelian subgroup C1 NOp 1

This journal is © The Royal Society of Chemistry 2014

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.530896	0.775196	0.982851
2	6	0	0.599285	1.172825	0.166371
3	6	0	-0.651319	-0.614686	1.251656
4	6	0	0.331341	-1.482634	0.639703
5	1	0	0.207367	-2.552382	0.800311
6	6	0	-0.160234	-1.338562	-1.350058
7	1	0	0.540555	-2.102515	-1.666227
8	6	0	-0.089227	0.009873	-1.772022
9	1	0	0.717820	0.469718	-2.324964
10	6	0	-1.523164	1.666070	1.449442
11	1	0	-1.443850	2.725727	1.225276
12	6	0	-2.581431	1.182321	2.200154
13	1	0	-3.332559	1.871556	2.575482
14	6	0	-2.699378	-0.196629	2.472482
15	1	0	-3.540135	-0.561121	3.055879
16	6	0	-1.757996	-1.088996	1.986189
17	1	0	-1.859277	-2.155358	2.168910
18	6	0	1.686043	-0.981690	0.524153
19	6	0	1.829536	0.402416	0.249183
20	6	0	3.114658	0.934706	0.005354
21	1	0	3.226941	1.992748	-0.213493
22	6	0	4.227101	0.110164	0.068814
23	1	0	5.216443	0.528418	-0.094330
24	6	0	4.085066	-1.265740	0.343107
25	1	0	4.965335	-1.900837	0.390786
26	6	0	2.826354	-1.809491	0.550291
27	1	0	2.710644	-2.871917	0.751557
28	6	0	-1.470091	0.499350	-1.940316
29	6	0	-1.612190	-1.694075	-1.329077
30	8	0	-2.344249	-0.540942	-1.559265
31	8	0	-2.133709	-2.759819	-1.130406
32	8	0	-1.892687	1.555690	-2.324740
33	6	0	0.698407	2.543767	-0.245593
34	7	0	0.803526	3.653062	-0.581426

Rotational constants (GHZ): 0.3914929 0.2664849 0.2437577

Standard basis: 6-31+G(d) (6D, 7F)

There are 459 symmetry adapted basis functions of A symmetry.

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

459 basis functions, 780 primitive gaussians, 459 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1864.4008800053 Hartrees.

This journal is © The Royal Society of Chemistry 2014

```
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Initial guess read from the read-write file:
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB+HF-LYP) =  -1011.05929351     A.U. after   11 cycles
```

```
            Convg  =    0.9914D-08            -V/T =  2.0094
            S**2   =   0.0000
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
    1          6          -0.000001947    0.000006032    0.000004986
    2          6          -0.000009453   -0.000031010    0.000117151
    3          6           0.000006508   -0.000000847    0.000000719
    4          6          -0.000010341    0.000017255    0.000002766
    5          1          -0.000001491   -0.000005340   -0.000006094
    6          6           0.000015705   -0.000009329   -0.000000899
    7          1          -0.000006435   -0.000012551   -0.000010158
    8          6          -0.000001793    0.000042120    0.000001803
    9          1           0.000003496    0.000006543   -0.000008004
   10          6          -0.000000236    0.000000995    0.000002197
   11          1          -0.000000694    0.000001223    0.000002314
   12          6          -0.000000918   -0.000002269    0.000002408
   13          1          -0.000001568   -0.000001078    0.000003172
   14          6          -0.000001043   -0.000003545    0.000003446
   15          1          -0.000001643   -0.000004268    0.000003455
   16          6          -0.000003700   -0.000001643    0.000002357
   17          1          -0.000000423   -0.000004396    0.000001497
   18          6          -0.000004237   -0.000005722   -0.000004480
   19          6           0.000004897    0.000003324    0.000003072
   20          6          -0.000003200    0.000004252    0.000000039
   21          1          -0.000000463    0.000005269   -0.000000117
   22          6           0.000000469    0.000002839    0.000002464
   23          1          -0.000000196    0.000004857   -0.000000649
   24          6           0.000000654    0.000002075   -0.000001805
   25          1           0.000000143    0.000001587   -0.000000528
   26          6           0.000000087    0.000001583   -0.000000252
   27          1           0.000000017   -0.000001444   -0.000000407
   28          6          -0.000005454   -0.000015515   -0.000000467
   29          6           0.000008710   -0.000001989   -0.000001577
   30          8           0.000002385   -0.000002331   -0.000001993
   31          8           0.000001667   -0.000004655   -0.000002991
   32          8          -0.000000263    0.000000481    0.000003462
   33          6           0.000009254    0.000004967   -0.000108805
   34          7           0.000001505    0.000002530   -0.000008082
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000117151 RMS     0.000017350


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Internal  Forces:  Max     0.000115830 RMS     0.000010160
 Search for a saddle point.
 Step number   6 out of a maximum of 195
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
```

This journal is © The Royal Society of Chemistry 2014

```
 Swaping is turned off.
 Update second derivatives using D2CorX and points  3  4  5  6
     Eigenvalues ---   -0.02264   0.00327   0.00573   0.00803
0.00997
     Eigenvalues ---    0.01221   0.01460   0.01520   0.01602
0.01646
     Eigenvalues ---    0.01734   0.01814   0.01904   0.01917
0.01950
     Eigenvalues ---    0.02029   0.02087   0.02174   0.02222
0.02284
     Eigenvalues ---    0.02396   0.02475   0.02492   0.02516
0.02714
     Eigenvalues ---    0.02759   0.02770   0.02778   0.03467
0.03997
     Eigenvalues ---    0.05469   0.06599   0.06973   0.07478
0.08533
     Eigenvalues ---    0.10372   0.11087   0.11157   0.11193
0.11822
     Eigenvalues ---    0.11898   0.12501   0.12521   0.12651
0.12705
     Eigenvalues ---    0.12907   0.14152   0.16386   0.17483
0.18104
     Eigenvalues ---    0.19142   0.19157   0.19203   0.19396
0.19564
     Eigenvalues ---    0.19763   0.20345   0.20980   0.23509
0.23958
     Eigenvalues ---    0.25131   0.25343   0.26456   0.27923
0.28538
     Eigenvalues ---    0.29516   0.30080   0.31015   0.31809
0.33484
     Eigenvalues ---    0.34194   0.35311   0.35873   0.35903
0.36040
     Eigenvalues ---    0.36126   0.36225   0.36265   0.36292
0.36350
     Eigenvalues ---    0.37237   0.38016   0.39089   0.40147
0.40785
     Eigenvalues ---    0.41735   0.42416   0.42890   0.44730
0.47343
     Eigenvalues ---    0.47621   0.50295   0.50637   0.88539
0.89747
     Eigenvalues ---
1.375151000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
 Eigenvectors required to have negative eigenvalues:
                           R1        R2        R3        R4        R5
          1           -0.05210   0.02431   0.14080   0.01800
0.39530
                           R6        R7        R8        R9        R10
          1            0.11840  -0.05449  -0.01585  -0.05723
0.18715
                           R11       R12       R13       R14       R15
          1            0.01985  -0.00750   0.43485   0.18905  -
0.05544
                           R16       R17       R18       R19       R20
          1            0.28785  -0.00780  -0.09671   0.17049  -
0.01253
                           R21       R22       R23       R24       R25
          1           -0.03369  -0.00835   0.15043  -0.00652  -
0.05558
                           R26       R27       R28       R29       R30
          1            0.03260  -0.00033  -0.01469   0.00002
0.01630
                           R31       R32       R33       R34       R35
          1           -0.00013  -0.01576  -0.00020   0.01992
0.01837
                           R36       R37       R38       R39       R40
          1            0.01812  -0.00013  -0.01401   0.00004
0.01530
                           R41       R42       R43       R44       R45
          1           -0.00006  -0.01506  -0.00014   0.00085
0.00170
```

This journal is © The Royal Society of Chemistry 2014

	R46	R47	R48	A1	A2
1	-0.00157	0.00221	-0.00063	0.02025	-0.01077
	A3	A4	A5	A6	A7
1	-0.00892	0.04596	0.01997	0.01161	0.02000
	A8	A9	A10	A11	A12
1	-0.00557	-0.01336	0.03233	0.05640	0.03016
	A13	A14	A15	A16	A17
1	0.06088	0.03658	0.02202	0.04539	0.00791
	A18	A19	A20	A21	A22
1	0.01970	-0.00652	0.00584	0.00067	0.00051
	A23	A24	A25	A26	A27
1	0.00293	-0.00344	-0.00239	0.00088	0.00153
	A28	A29	A30	A31	A32
1	0.00492	-0.00637	0.00143	0.01919	-0.01425
	A33	A34	A35	A36	A37
1	-0.00403	0.02279	-0.01272	-0.00946	-0.00623
	A38	A39	A40	A41	A42
1	0.00620	-0.00001	0.00088	0.00229	-0.00316
	A43	A44	A45	A46	A47
1	-0.00224	0.00041	0.00184	0.00465	-0.00601
	A48	A49	A50	A51	A52
1	0.00131	-0.00185	0.00289	-0.00105	-0.00638
	A53	A54	A55	A56	A57
1	0.00428	0.00224	-0.01406	0.00096	0.01942
	D1	D2	D3	D4	D5
1	0.16175	-0.02825	0.15073	-0.03927	0.00462
	D6	D7	D8	D9	D10
1	-0.00689	0.01499	0.00348	0.00817	0.00867
	D11	D12	D13	D14	D15
1	-0.00411	-0.00361	-0.16309	-0.15158	0.02729
	D16	D17	D18	D19	D20
1	0.03880	0.05122	-0.16471	0.06377	-0.15216
	D21	D22	D23	D24	D25
1	-0.00090	0.00222	-0.01512	-0.01201	0.16278
	D26	D27	D28	D29	D30

```
          1              0.15252  -0.05508  -0.06535   0.00422
0.16719
                           D31       D32       D33       D34       D35
          1             -0.16761  -0.00464  -0.14189  -0.14896
0.02972
                           D36       D37       D38       D39       D40
          1              0.02266  -0.02112  -0.01995   0.13774
0.13891
                           D41       D42       D43       D44       D45
          1              0.00019   0.00097   0.00074   0.00153  -
0.00052
                           D46       D47       D48       D49       D50
          1              0.00140   0.00029   0.00221  -0.00141  -
0.00459
                           D51       D52       D53       D54       D55
          1              0.00049  -0.00270  -0.00185  -0.01262
0.00729
                           D56       D57       D58       D59       D60
          1             -0.00347   0.01318   0.00993   0.00134  -
0.00191
                           D61       D62       D63       D64       D65
          1             -0.00746  -0.00966   0.00545   0.00324
0.00100
                           D66       D67       D68       D69       D70
          1             -0.00070  -0.00128  -0.00298   0.00092  -
0.00131
                           D71       D72       D73       D74       D75
          1             -0.00078  -0.00301   0.00096   0.00432  -
0.00127
                           D76       D77       D78       D79       D80
          1              0.00209   0.04242   0.04140  -0.04709  -
0.04057
 RFO step:  Lambda0=4.520193587D-09 Lambda=-1.49399120D-07.
 Linear search not attempted -- option 19 set.
 Iteration  1 RMS(Cart)=  0.00033471 RMS(Int)=  0.00000008
 Iteration  2 RMS(Cart)=  0.00000011 RMS(Int)=  0.00000002
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                 (Linear)    (Quad)   (Total)
    R1        2.73981   0.00000   0.00000   0.00003   0.00003
2.73984
    R2        2.68483   0.00000   0.00000   0.00000   0.00000
2.68483
    R3        5.46719  -0.00001   0.00000  -0.00064  -0.00064
5.46655
    R4        2.66977   0.00000   0.00000  -0.00001  -0.00001
2.66976
    R5        4.46547   0.00000   0.00000  -0.00112  -0.00112
4.46434
    R6        4.89697  -0.00003   0.00000  -0.00061  -0.00061
4.89636
```

This journal is © The Royal Society of Chemistry 2014

R7	2.74753	0.00000	0.00000	0.00002	0.00002
2.74755					
R8	2.71162	0.00012	0.00000	0.00052	0.00052
2.71215					
R9	2.73419	-0.00001	0.00000	-0.00011	-0.00011
2.73408					
R10	5.18697	0.00002	0.00000	0.00078	0.00078
5.18776					
R11	2.66528	0.00000	0.00000	0.00003	0.00003
2.66531					
R12	2.05757	0.00000	0.00000	-0.00003	-0.00003
2.05754					
R13	3.88271	0.00000	0.00000	0.00119	0.00119
3.88390					
R14	4.52957	0.00002	0.00000	0.00095	0.00095
4.53052					
R15	2.73816	0.00000	0.00000	-0.00007	-0.00007
2.73808					
R16	4.71773	-0.00001	0.00000	0.00084	0.00084
4.71856					
R17	2.04815	-0.00001	0.00000	-0.00005	-0.00005
2.04810					
R18	2.67339	0.00000	0.00000	-0.00007	-0.00007
2.67333					
R19	5.01713	-0.00001	0.00000	0.00020	0.00020
5.01733					
R20	2.82513	-0.00001	0.00000	-0.00013	-0.00013
2.82500					
R21	5.12884	-0.00002	0.00000	-0.00036	-0.00036
5.12848					
R22	2.04276	0.00001	0.00000	0.00003	0.00003
2.04279					
R23	5.31850	0.00001	0.00000	-0.00035	-0.00035
5.31815					
R24	2.78675	0.00001	0.00000	0.00012	0.00012
2.78687					
R25	5.30023	0.00001	0.00000	0.00041	0.00041
5.30064					
R26	5.55008	0.00000	0.00000	-0.00013	-0.00013
5.54995					
R27	2.05226	0.00000	0.00000	0.00000	0.00000
2.05226					
R28	2.61678	0.00000	0.00000	0.00000	0.00000
2.61678					
R29	2.05286	0.00000	0.00000	0.00000	0.00000
2.05286					
R30	2.66550	0.00000	0.00000	0.00001	0.00001
2.66551					
R31	2.05284	0.00000	0.00000	0.00000	0.00000
2.05284					
R32	2.61780	0.00000	0.00000	-0.00002	-0.00002
2.61778					

This journal is © The Royal Society of Chemistry 2014

R33	2.05344	0.00000	0.00000	0.00000	0.00000
2.05344					
R34	2.68045	-0.00001	0.00000	-0.00001	-0.00001
2.68044					
R35	2.66327	0.00000	0.00000	0.00002	0.00002
2.66329					
R36	2.66868	0.00000	0.00000	-0.00001	-0.00001
2.66867					
R37	2.05273	0.00000	0.00000	0.00000	0.00000
2.05273					
R38	2.61945	0.00000	0.00000	0.00000	0.00000
2.61946					
R39	2.05307	0.00000	0.00000	0.00000	0.00000
2.05307					
R40	2.66480	0.00000	0.00000	0.00000	0.00000
2.66480					
R41	2.05320	0.00000	0.00000	0.00000	0.00000
2.05320					
R42	2.62049	0.00000	0.00000	-0.00001	-0.00001
2.62048					
R43	2.05507	0.00000	0.00000	0.00000	0.00000
2.05507					
R44	2.66683	0.00000	0.00000	-0.00009	-0.00009
2.66674					
R45	2.26942	0.00000	0.00000	-0.00001	-0.00001
2.26941					
R46	2.61754	0.00000	0.00000	0.00008	0.00008
2.61762					
R47	2.27338	0.00000	0.00000	0.00000	0.00000
2.27339					
R48	2.19921	0.00001	0.00000	-0.00001	-0.00001
2.19921					
A1	2.02742	-0.00001	0.00000	-0.00004	-0.00004
2.02738					
A2	2.16583	0.00000	0.00000	0.00003	0.00003
2.16586					
A3	2.08847	0.00000	0.00000	0.00000	0.00000
2.08847					
A4	2.07396	0.00000	0.00000	-0.00004	-0.00004
2.07392					
A5	2.06866	0.00002	0.00000	-0.00010	-0.00010
2.06856					
A6	2.05348	-0.00002	0.00000	-0.00014	-0.00014
2.05333					
A7	2.03673	0.00001	0.00000	0.00002	0.00002
2.03675					
A8	2.08751	0.00000	0.00000	0.00000	0.00000
2.08751					
A9	2.15488	0.00000	0.00000	-0.00001	-0.00001
2.15488					
A10	2.03717	0.00000	0.00000	0.00010	0.00010
2.03728					

This journal is © The Royal Society of Chemistry 2014

A11	2.05027	0.00000	0.00000	0.00011	0.00011
2.05038					
A12	2.04641	0.00000	0.00000	0.00011	0.00011
2.04652					
A13	2.15602	0.00000	0.00000	0.00014	0.00014
2.15616					
A14	2.05381	-0.00001	0.00000	0.00016	0.00016
2.05396					
A15	1.85417	0.00001	0.00000	0.00011	0.00011
1.85428					
A16	2.20870	0.00000	0.00000	-0.00015	-0.00015
2.20855					
A17	1.87907	-0.00001	0.00000	-0.00008	-0.00008
1.87899					
A18	2.09383	0.00000	0.00000	-0.00011	-0.00012
2.09372					
A19	2.08957	0.00000	0.00000	0.00000	0.00000
2.08957					
A20	2.08923	0.00000	0.00000	0.00000	0.00000
2.08922					
A21	2.10433	0.00000	0.00000	0.00000	0.00000
2.10434					
A22	2.08758	0.00000	0.00000	-0.00001	-0.00001
2.08757					
A23	2.10609	0.00000	0.00000	0.00001	0.00001
2.10610					
A24	2.08948	0.00000	0.00000	0.00000	0.00000
2.08948					
A25	2.09027	0.00000	0.00000	0.00000	0.00000
2.09027					
A26	2.10036	0.00000	0.00000	-0.00001	-0.00001
2.10036					
A27	2.09247	0.00000	0.00000	0.00000	0.00000
2.09248					
A28	2.09371	0.00000	0.00000	0.00000	0.00000
2.09371					
A29	2.08372	0.00000	0.00000	-0.00001	-0.00001
2.08371					
A30	2.10574	0.00000	0.00000	0.00001	0.00001
2.10575					
A31	2.03465	0.00000	0.00000	0.00002	0.00002
2.03467					
A32	2.15546	0.00000	0.00000	-0.00001	-0.00001
2.15545					
A33	2.08851	0.00000	0.00000	0.00001	0.00001
2.08852					
A34	2.02918	0.00001	0.00000	-0.00004	-0.00004
2.02914					
A35	2.16573	0.00000	0.00000	0.00004	0.00004
2.16577					
A36	2.08671	0.00000	0.00000	0.00000	0.00000
2.08671					

This journal is © The Royal Society of Chemistry 2014

A37	2.08976	0.00000	0.00000	0.00000	0.00000	2.08976
A38	2.09232	0.00000	0.00000	0.00000	0.00000	2.09232
A39	2.10094	0.00000	0.00000	0.00000	0.00000	2.10094
A40	2.08856	0.00000	0.00000	-0.00001	-0.00001	2.08856
A41	2.10420	0.00000	0.00000	0.00001	0.00001	2.10420
A42	2.09042	0.00000	0.00000	0.00000	0.00000	2.09043
A43	2.09124	0.00000	0.00000	0.00000	0.00000	2.09125
A44	2.09796	0.00000	0.00000	0.00000	0.00000	2.09796
A45	2.09398	0.00000	0.00000	0.00000	0.00000	2.09398
A46	2.09594	0.00000	0.00000	0.00000	0.00000	2.09594
A47	2.08423	0.00000	0.00000	-0.00001	-0.00001	2.08422
A48	2.10286	0.00000	0.00000	0.00001	0.00001	2.10287
A49	1.88024	0.00000	0.00000	0.00002	0.00002	1.88026
A50	2.28895	0.00000	0.00000	-0.00005	-0.00005	2.28889
A51	2.11398	-0.00001	0.00000	0.00004	0.00004	2.11402
A52	1.88914	0.00000	0.00000	-0.00002	-0.00002	1.88911
A53	2.25753	0.00000	0.00000	0.00007	0.00007	2.25759
A54	2.13629	0.00000	0.00000	-0.00004	-0.00004	2.13625
A55	1.90835	0.00000	0.00000	-0.00001	-0.00001	1.90834
A56	3.16075	0.00001	0.00000	0.00007	0.00007	3.16081
A57	3.12264	0.00000	0.00000	-0.00010	-0.00010	3.12254
D1	-0.55077	0.00000	0.00000	-0.00026	-0.00026	-0.55103
D2	3.03680	0.00001	0.00000	0.00046	0.00046	3.03726
D3	2.64927	0.00000	0.00000	-0.00011	-0.00011	2.64916
D4	-0.04635	0.00001	0.00000	0.00062	0.00062	-0.04574
D5	-0.04194	0.00001	0.00000	0.00031	0.00031	-0.04163

This journal is © The Royal Society of Chemistry 2014

D6	-3.09023	0.00000	0.00000	0.00018	0.00018	-3.09005
D7	3.04396	0.00000	0.00000	0.00016	0.00016	3.04412
D8	-0.00433	0.00000	0.00000	0.00003	0.00003	-0.00430
D9	-0.03624	0.00000	0.00000	-0.00015	-0.00015	-0.03639
D10	3.11666	0.00000	0.00000	-0.00017	-0.00017	3.11648
D11	-3.11747	0.00000	0.00000	0.00001	0.00001	-3.11746
D12	0.03542	0.00000	0.00000	-0.00001	-0.00001	0.03542
D13	0.55182	0.00000	0.00000	0.00019	0.00019	0.55201
D14	-2.65029	0.00000	0.00000	0.00008	0.00008	-2.65022
D15	-3.03189	0.00000	0.00000	-0.00051	-0.00051	-3.03241
D16	0.04918	0.00000	0.00000	-0.00063	-0.00063	0.04855
D17	-3.08447	0.00000	0.00000	0.00032	0.00032	-3.08415
D18	0.63149	0.00000	0.00000	-0.00028	-0.00028	0.63121
D19	-0.04014	0.00000	0.00000	0.00046	0.00046	-0.03968
D20	-2.60736	0.00000	0.00000	-0.00014	-0.00014	-2.60750
D21	-0.03143	0.00000	0.00000	-0.00003	-0.00003	-0.03145
D22	3.11566	0.00000	0.00000	0.00003	0.00003	3.11569
D23	-3.07307	0.00000	0.00000	-0.00017	-0.00017	-3.07325
D24	0.07402	0.00000	0.00000	-0.00011	-0.00011	0.07390
D25	-0.63022	0.00000	0.00000	0.00020	0.00020	-0.63002
D26	2.61441	0.00000	0.00000	0.00010	0.00010	2.61451
D27	3.08880	0.00000	0.00000	-0.00040	-0.00040	3.08840
D28	0.05024	0.00000	0.00000	-0.00050	-0.00050	0.04974
D29	-0.16050	0.00000	0.00000	0.00111	0.00111	-0.15939
D30	2.50458	-0.00001	0.00000	0.00033	0.00033	2.50491
D31	-2.61530	0.00001	0.00000	0.00050	0.00050	-2.61479

This journal is © The Royal Society of Chemistry 2014

D32	0.04978	-0.00001	0.00000	-0.00028	-0.00028	0.04951
D33	-2.63308	0.00001	0.00000	-0.00034	-0.00034	-2.63342
D34	0.53138	0.00000	0.00000	-0.00035	-0.00035	0.53103
D35	-0.13103	0.00000	0.00000	0.00021	0.00021	-0.13081
D36	3.03343	0.00000	0.00000	0.00021	0.00021	3.03364
D37	0.04568	0.00001	0.00000	0.00026	0.00026	0.04593
D38	-3.09016	0.00001	0.00000	0.00026	0.00026	-3.08991
D39	2.74792	-0.00001	0.00000	-0.00048	-0.00048	2.74744
D40	-0.38792	-0.00001	0.00000	-0.00048	-0.00048	-0.38839
D41	3.11965	0.00000	0.00000	-0.00001	-0.00001	3.11964
D42	-0.03121	0.00000	0.00000	-0.00002	-0.00002	-0.03123
D43	-0.01054	0.00000	0.00000	-0.00003	-0.00003	-0.01057
D44	3.12178	0.00000	0.00000	-0.00004	-0.00004	3.12175
D45	-3.13257	0.00000	0.00000	0.00001	0.00001	-3.13256
D46	-0.00476	0.00000	0.00000	0.00002	0.00002	-0.00474
D47	-0.00025	0.00000	0.00000	0.00000	0.00000	-0.00026
D48	3.12755	0.00000	0.00000	0.00001	0.00001	3.12756
D49	0.03622	0.00000	0.00000	0.00000	0.00000	0.03623
D50	-3.11094	0.00000	0.00000	-0.00005	-0.00005	-3.11099
D51	-3.11917	0.00000	0.00000	0.00002	0.00002	-3.11916
D52	0.01685	0.00000	0.00000	-0.00004	-0.00004	0.01681
D53	0.04073	0.00001	0.00000	-0.00018	-0.00018	0.04055
D54	-3.04325	0.00000	0.00000	-0.00007	-0.00007	-3.04332
D55	3.08345	0.00000	0.00000	-0.00008	-0.00008	3.08337
D56	-0.00053	0.00000	0.00000	0.00003	0.00003	-0.00050
D57	3.06523	0.00000	0.00000	0.00009	0.00009	3.06532

```
   D58       -0.09531   0.00000   0.00000   0.00008   0.00008  -
0.09523
   D59        0.02970   0.00000   0.00000  -0.00002  -0.00002
0.02968
   D60       -3.13084   0.00000   0.00000  -0.00003  -0.00003  -
3.13087
   D61        0.05373   0.00000   0.00000   0.00010   0.00010
0.05383
   D62       -3.10696   0.00000   0.00000   0.00010   0.00010  -
3.10686
   D63        3.13293   0.00000   0.00000  -0.00002  -0.00002
3.13291
   D64       -0.02776   0.00000   0.00000  -0.00002  -0.00002  -
0.02778
   D65       -3.11440   0.00000   0.00000   0.00000   0.00000  -
3.11440
   D66        0.02723   0.00000   0.00000   0.00001   0.00001
0.02723
   D67        0.00797   0.00000   0.00000   0.00000   0.00000
0.00797
   D68       -3.13359   0.00000   0.00000   0.00000   0.00000  -
3.13358
   D69       -3.14079   0.00000   0.00000   0.00001   0.00001  -
3.14078
   D70        0.00209   0.00000   0.00000   0.00000   0.00000
0.00209
   D71        0.00084   0.00000   0.00000   0.00001   0.00001
0.00085
   D72       -3.13947   0.00000   0.00000   0.00001   0.00001  -
3.13947
   D73       -0.03067   0.00000   0.00000   0.00000   0.00000  -
0.03067
   D74        3.13007   0.00000   0.00000   0.00001   0.00001
3.13008
   D75        3.11220   0.00000   0.00000   0.00000   0.00000
3.11220
   D76       -0.01024   0.00000   0.00000   0.00001   0.00001  -
0.01023
   D77       -0.13117   0.00000   0.00000  -0.00012  -0.00012  -
0.13129
   D78        3.00536   0.00000   0.00000  -0.00012  -0.00012
3.00524
   D79        0.16257   0.00000   0.00000  -0.00006  -0.00006
0.16251
   D80       -2.99996   0.00000   0.00000  -0.00005  -0.00005  -
3.00001
         Item               Value     Threshold  Converged?
 Maximum Force            0.000116     0.000450     YES
 RMS     Force            0.000010     0.000300     YES
 Maximum Displacement     0.001499     0.001800     YES
 RMS     Displacement     0.000335     0.001200     YES
 Predicted change in Energy=-7.243918D-08
```

This journal is © The Royal Society of Chemistry 2014

Optimization completed.
-- Stationary point found.

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.4498	-DE/DX = 0.0
R2	R(1,3)	1.4207	-DE/DX = 0.0
R3	R(1,8)	2.8931	-DE/DX = 0.0
R4	R(1,10)	1.4128	-DE/DX = 0.0
R5	R(2,8)	2.363	-DE/DX = 0.0
R6	R(2,9)	2.5914	-DE/DX = 0.0
R7	R(2,19)	1.4539	-DE/DX = 0.0
R8	R(2,33)	1.4349	-DE/DX = 0.0001
R9	R(3,4)	1.4469	-DE/DX = 0.0
R10	R(3,6)	2.7448	-DE/DX = 0.0
R11	R(3,16)	1.4104	-DE/DX = 0.0
R12	R(4,5)	1.0888	-DE/DX = 0.0
R13	R(4,6)	2.0546	-DE/DX = 0.0
R14	R(4,7)	2.3969	-DE/DX = 0.0
R15	R(4,18)	1.449	-DE/DX = 0.0
R16	R(5,6)	2.4965	-DE/DX = 0.0
R17	R(6,7)	1.0838	-DE/DX = 0.0
R18	R(6,8)	1.4147	-DE/DX = 0.0
R19	R(6,18)	2.655	-DE/DX = 0.0
R20	R(6,29)	1.495	-DE/DX = 0.0

This journal is © The Royal Society of Chemistry 2014

```
 ! R21   R(7,18)                2.7141         -DE/DX =    0.0
!
 ! R22   R(8,9)                 1.081          -DE/DX =    0.0
!
 ! R23   R(8,19)                2.8144         -DE/DX =    0.0
!
 ! R24   R(8,28)                1.4747         -DE/DX =    0.0
!
 ! R25   R(9,19)                2.8048         -DE/DX =    0.0
!
 ! R26   R(9,33)                2.937          -DE/DX =    0.0
!
 ! R27   R(10,11)               1.086          -DE/DX =    0.0
!
 ! R28   R(10,12)               1.3847         -DE/DX =    0.0
!
 ! R29   R(12,13)               1.0863         -DE/DX =    0.0
!
 ! R30   R(12,14)               1.4105         -DE/DX =    0.0
!
 ! R31   R(14,15)               1.0863         -DE/DX =    0.0
!
 ! R32   R(14,16)               1.3853         -DE/DX =    0.0
!
 ! R33   R(16,17)               1.0866         -DE/DX =    0.0
!
 ! R34   R(18,19)               1.4184         -DE/DX =    0.0
!
 ! R35   R(18,26)               1.4093         -DE/DX =    0.0
!
 ! R36   R(19,20)               1.4122         -DE/DX =    0.0
!
 ! R37   R(20,21)               1.0863         -DE/DX =    0.0
!
 ! R38   R(20,22)               1.3862         -DE/DX =    0.0
!
 ! R39   R(22,23)               1.0864         -DE/DX =    0.0
!
 ! R40   R(22,24)               1.4101         -DE/DX =    0.0
!
 ! R41   R(24,25)               1.0865         -DE/DX =    0.0
!
 ! R42   R(24,26)               1.3867         -DE/DX =    0.0
!
 ! R43   R(26,27)               1.0875         -DE/DX =    0.0
!
 ! R44   R(28,30)               1.4112         -DE/DX =    0.0
!
 ! R45   R(28,32)               1.2009         -DE/DX =    0.0
!
 ! R46   R(29,30)               1.3851         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R47   R(29,31)              1.203          -DE/DX =    0.0
!
 ! R48   R(33,34)              1.1638         -DE/DX =    0.0
!
 ! A1    A(2,1,3)             116.1624        -DE/DX =    0.0
!
 ! A2    A(2,1,10)            124.0932        -DE/DX =    0.0
!
 ! A3    A(3,1,10)            119.6608        -DE/DX =    0.0
!
 ! A4    A(1,2,19)            118.8289        -DE/DX =    0.0
!
 ! A5    A(1,2,33)            118.5257        -DE/DX =    0.0
!
 ! A6    A(19,2,33)           117.6555        -DE/DX =    0.0
!
 ! A7    A(1,3,4)             116.6961        -DE/DX =    0.0
!
 ! A8    A(1,3,16)            119.6057        -DE/DX =    0.0
!
 ! A9    A(4,3,16)            123.4658        -DE/DX =    0.0
!
 ! A10   A(3,4,5)             116.7215        -DE/DX =    0.0
!
 ! A11   A(3,4,18)            117.4717        -DE/DX =    0.0
!
 ! A12   A(5,4,18)            117.2508        -DE/DX =    0.0
!
 ! A13   A(7,6,8)             123.5307        -DE/DX =    0.0
!
 ! A14   A(7,6,29)            117.6744        -DE/DX =    0.0
!
 ! A15   A(8,6,29)            106.2362        -DE/DX =    0.0
!
 ! A16   A(6,8,9)             126.5492        -DE/DX =    0.0
!
 ! A17   A(6,8,28)            107.6627        -DE/DX =    0.0
!
 ! A18   A(9,8,28)            119.9679        -DE/DX =    0.0
!
 ! A19   A(1,10,11)           119.7235        -DE/DX =    0.0
!
 ! A20   A(1,10,12)           119.7038        -DE/DX =    0.0
!
 ! A21   A(11,10,12)          120.5695        -DE/DX =    0.0
!
 ! A22   A(10,12,13)          119.6093        -DE/DX =    0.0
!
 ! A23   A(10,12,14)          120.6703        -DE/DX =    0.0
!
 ! A24   A(13,12,14)          119.7184        -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A25   A(12,14,15)           119.7637         -DE/DX =    0.0
!
 ! A26   A(12,14,16)           120.3419         -DE/DX =    0.0
!
 ! A27   A(15,14,16)           119.8897         -DE/DX =    0.0
!
 ! A28   A(3,16,14)            119.9608         -DE/DX =    0.0
!
 ! A29   A(3,16,17)            119.3884         -DE/DX =    0.0
!
 ! A30   A(14,16,17)           120.65           -DE/DX =    0.0
!
 ! A31   A(4,18,19)            116.577          -DE/DX =    0.0
!
 ! A32   A(4,18,26)            123.499          -DE/DX =    0.0
!
 ! A33   A(19,18,26)           119.6629         -DE/DX =    0.0
!
 ! A34   A(2,19,18)            116.2635         -DE/DX =    0.0
!
 ! A35   A(2,19,20)            124.0872         -DE/DX =    0.0
!
 ! A36   A(18,19,20)           119.5597         -DE/DX =    0.0
!
 ! A37   A(19,20,21)           119.7344         -DE/DX =    0.0
!
 ! A38   A(19,20,22)           119.8814         -DE/DX =    0.0
!
 ! A39   A(21,20,22)           120.3751         -DE/DX =    0.0
!
 ! A40   A(20,22,23)           119.6658         -DE/DX =    0.0
!
 ! A41   A(20,22,24)           120.5617         -DE/DX =    0.0
!
 ! A42   A(23,22,24)           119.7725         -DE/DX =    0.0
!
 ! A43   A(22,24,25)           119.8194         -DE/DX =    0.0
!
 ! A44   A(22,24,26)           120.2042         -DE/DX =    0.0
!
 ! A45   A(25,24,26)           119.9763         -DE/DX =    0.0
!
 ! A46   A(18,26,24)           120.0887         -DE/DX =    0.0
!
 ! A47   A(18,26,27)           119.4175         -DE/DX =    0.0
!
 ! A48   A(24,26,27)           120.4848         -DE/DX =    0.0
!
 ! A49   A(8,28,30)            107.73           -DE/DX =    0.0
!
 ! A50   A(8,28,32)            131.147          -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A51   A(30,28,32)           121.1222         -DE/DX =    0.0
!
 ! A52   A(6,29,30)            108.2396         -DE/DX =    0.0
!
 ! A53   A(6,29,31)            129.3468         -DE/DX =    0.0
!
 ! A54   A(30,29,31)           122.4006         -DE/DX =    0.0
!
 ! A55   A(28,30,29)           109.3404         -DE/DX =    0.0
!
 ! A56   L(2,33,34,1,-1)       181.0974         -DE/DX =    0.0
!
 ! A57   L(2,33,34,1,-2)       178.9142         -DE/DX =    0.0
!
 ! D1    D(3,1,2,19)           -31.5565         -DE/DX =    0.0
!
 ! D2    D(3,1,2,33)           173.9959         -DE/DX =    0.0
!
 ! D3    D(10,1,2,19)          151.7918         -DE/DX =    0.0
!
 ! D4    D(10,1,2,33)           -2.6558         -DE/DX =    0.0
!
 ! D5    D(2,1,3,4)             -2.4031         -DE/DX =    0.0
!
 ! D6    D(2,1,3,16)          -177.0572         -DE/DX =    0.0
!
 ! D7    D(10,1,3,4)           174.4062         -DE/DX =    0.0
!
 ! D8    D(10,1,3,16)           -0.2479         -DE/DX =    0.0
!
 ! D9    D(2,1,10,11)           -2.0764         -DE/DX =    0.0
!
 ! D10   D(2,1,10,12)          178.5712         -DE/DX =    0.0
!
 ! D11   D(3,1,10,11)         -178.6179         -DE/DX =    0.0
!
 ! D12   D(3,1,10,12)            2.0297         -DE/DX =    0.0
!
 ! D13   D(1,2,19,18)           31.6168         -DE/DX =    0.0
!
 ! D14   D(1,2,19,20)         -151.8506         -DE/DX =    0.0
!
 ! D15   D(33,2,19,18)        -173.7146         -DE/DX =    0.0
!
 ! D16   D(33,2,19,20)           2.818          -DE/DX =    0.0
!
 ! D17   D(1,3,4,5)           -176.7274         -DE/DX =    0.0
!
 ! D18   D(1,3,4,18)            36.1817         -DE/DX =    0.0
!
 ! D19   D(16,3,4,5)             -2.2998         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D20   D(16,3,4,18)         -149.3907         -DE/DX =    0.0
!
 ! D21   D(1,3,16,14)           -1.8005         -DE/DX =    0.0
!
 ! D22   D(1,3,16,17)          178.5143         -DE/DX =    0.0
!
 ! D23   D(4,3,16,14)         -176.0741         -DE/DX =    0.0
!
 ! D24   D(4,3,16,17)            4.2408         -DE/DX =    0.0
!
 ! D25   D(3,4,18,19)          -36.1091         -DE/DX =    0.0
!
 ! D26   D(3,4,18,26)          149.7947         -DE/DX =    0.0
!
 ! D27   D(5,4,18,19)          176.975          -DE/DX =    0.0
!
 ! D28   D(5,4,18,26)            2.8788         -DE/DX =    0.0
!
 ! D29   D(7,6,8,9)              -9.1958         -DE/DX =    0.0
!
 ! D30   D(7,6,8,28)           143.5019         -DE/DX =    0.0
!
 ! D31   D(29,6,8,9)          -149.8454         -DE/DX =    0.0
!
 ! D32   D(29,6,8,28)            2.8524         -DE/DX =    0.0
!
 ! D33   D(7,6,29,30)         -150.8645         -DE/DX =    0.0
!
 ! D34   D(7,6,29,31)           30.4457         -DE/DX =    0.0
!
 ! D35   D(8,6,29,30)           -7.5072         -DE/DX =    0.0
!
 ! D36   D(8,6,29,31)          173.8029         -DE/DX =    0.0
!
 ! D37   D(6,8,28,30)            2.617          -DE/DX =    0.0
!
 ! D38   D(6,8,28,32)         -177.0532         -DE/DX =    0.0
!
 ! D39   D(9,8,28,30)          157.4442         -DE/DX =    0.0
!
 ! D40   D(9,8,28,32)          -22.2259         -DE/DX =    0.0
!
 ! D41   D(1,10,12,13)         178.7428         -DE/DX =    0.0
!
 ! D42   D(1,10,12,14)          -1.7882         -DE/DX =    0.0
!
 ! D43   D(11,10,12,13)         -0.604          -DE/DX =    0.0
!
 ! D44   D(11,10,12,14)        178.865          -DE/DX =    0.0
!
 ! D45   D(10,12,14,15)       -179.483          -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D46   D(10,12,14,16)         -0.2729         -DE/DX =    0.0
!
 ! D47   D(13,12,14,15)         -0.0146         -DE/DX =    0.0
!
 ! D48   D(13,12,14,16)        179.1956         -DE/DX =    0.0
!
 ! D49   D(12,14,16,3)           2.0753         -DE/DX =    0.0
!
 ! D50   D(12,14,16,17)       -178.2436         -DE/DX =    0.0
!
 ! D51   D(15,14,16,3)        -178.7156         -DE/DX =    0.0
!
 ! D52   D(15,14,16,17)          0.9656         -DE/DX =    0.0
!
 ! D53   D(4,18,19,2)            2.3336         -DE/DX =    0.0
!
 ! D54   D(4,18,19,20)        -174.3652         -DE/DX =    0.0
!
 ! D55   D(26,18,19,2)         176.6687         -DE/DX =    0.0
!
 ! D56   D(26,18,19,20)         -0.0301         -DE/DX =    0.0
!
 ! D57   D(4,18,26,24)         175.6247         -DE/DX =    0.0
!
 ! D58   D(4,18,26,27)          -5.4608         -DE/DX =    0.0
!
 ! D59   D(19,18,26,24)          1.7017         -DE/DX =    0.0
!
 ! D60   D(19,18,26,27)       -179.3839         -DE/DX =    0.0
!
 ! D61   D(2,19,20,21)           3.0786         -DE/DX =    0.0
!
 ! D62   D(2,19,20,22)        -178.0156         -DE/DX =    0.0
!
 ! D63   D(18,19,20,21)        179.5037         -DE/DX =    0.0
!
 ! D64   D(18,19,20,22)         -1.5905         -DE/DX =    0.0
!
 ! D65   D(19,20,22,23)       -178.4419         -DE/DX =    0.0
!
 ! D66   D(19,20,22,24)          1.56           -DE/DX =    0.0
!
 ! D67   D(21,20,22,23)          0.4568         -DE/DX =    0.0
!
 ! D68   D(21,20,22,24)       -179.5414         -DE/DX =    0.0
!
 ! D69   D(20,22,24,25)       -179.954          -DE/DX =    0.0
!
 ! D70   D(20,22,24,26)          0.1195         -DE/DX =    0.0
!
 ! D71   D(23,22,24,25)          0.0479         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D72   D(23,22,24,26)       -179.8786         -DE/DX =    0.0
!
 ! D73   D(22,24,26,18)         -1.7575         -DE/DX =    0.0
!
 ! D74   D(22,24,26,27)        179.3398         -DE/DX =    0.0
!
 ! D75   D(25,24,26,18)        178.3162         -DE/DX =    0.0
!
 ! D76   D(25,24,26,27)         -0.5866         -DE/DX =    0.0
!
 ! D77   D(8,28,30,29)           -7.5157         -DE/DX =    0.0
!
 ! D78   D(32,28,30,29)        172.1942         -DE/DX =    0.0
!
 ! D79   D(6,29,30,28)           9.3147         -DE/DX =    0.0
!
 ! D80   D(31,29,30,28)       -171.8852         -DE/DX =    0.0
!
 ---------------------------------------------------------------------
-----------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.559656    1.134053   -0.760894
    2          6             0        0.534139    0.448118   -1.420563
    3          6             0       -0.563909    1.085797    0.659030
    4          6             0        0.488312    0.315954    1.286416
    5          1             0        0.453901    0.233081    2.371530
    6          6             0       -0.011765   -1.601589    0.743735
    7          1             0        0.750622   -2.065494    1.358755
    8          6             0       -0.053157   -1.712798   -0.665979
    9          1             0        0.713200   -2.134296   -1.301246
   10          6             0       -1.623233    1.767069   -1.442108
   11          1             0       -1.632427    1.784872   -2.527931
   12          6             0       -2.638118    2.371198   -0.719234
   13          1             0       -3.444487    2.875245   -1.244416
   14          6             0       -2.640820    2.328847    0.690651
   15          1             0       -3.448755    2.800511    1.242787
   16          6             0       -1.627809    1.675303    1.373063
   17          1             0       -1.639909    1.615181    2.457965
   18          6             0        1.796586    0.340647    0.664062
   19          6             0        1.824317    0.382063   -0.753493
   20          6             0        3.060755    0.287283   -1.429188
   21          1             0        3.084545    0.310556   -2.514935
   22          6             0        4.238071    0.188075   -0.704268
   23          1             0        5.189204    0.140938   -1.227216
```

24	6	0	4.211109	0.147845	0.705050
25	1	0	5.141266	0.070715	1.261246
26	6	0	3.001979	0.204872	1.381586
27	1	0	2.975156	0.163421	2.467959
28	6	0	-1.469900	-1.795264	-1.066895
29	6	0	-1.429005	-1.688146	1.211651
30	8	0	-2.254536	-1.671278	0.099524
31	8	0	-1.859942	-1.740754	2.333608
32	8	0	-1.978830	-1.944199	-2.144408
33	6	0	0.518877	0.352191	-2.852201
34	7	0	0.531357	0.272627	-4.013184

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.449847	0.000000			
3	C	1.420749	2.436606	0.000000		
4	C	2.441106	2.710591	1.446873	0.000000	
5	H	3.413375	3.799032	2.166961	1.088818	0.000000
6	C	3.169831	3.030428	2.744828	2.054642	2.496513
7	H	4.055471	3.753628	3.485433	2.396943	2.529270
8	C	2.893115	2.363022	3.138256	2.867207	3.642803
9	H	3.548838	2.591363	3.980287	3.570756	4.377328
10	C	1.412784	2.528705	2.449710	3.742887	4.605588
11	H	2.167216	2.776181	3.433243	4.604834	5.546669
12	C	2.419146	3.775356	2.802537	4.245142	4.866719
13	H	3.404085	4.663844	3.888825	5.331228	5.937468
14	C	2.804596	4.251439	2.420689	3.768043	4.098157
15	H	3.890849	5.337661	3.406369	4.655687	4.805880
16	C	2.446972	3.739565	1.410406	2.516606	2.722215
17	H	3.429210	4.596900	2.161988	2.754966	2.510321
18	C	2.865636	2.439464	2.475320	1.448970	2.174815
19	C	2.499775	1.453928	2.862532	2.439367	3.415554
20	C	3.777699	2.531744	4.258693	3.740694	4.609130
21	H	4.127349	2.778695	4.897578	4.603338	5.550120
22	C	4.890426	3.781509	5.071834	4.247336	4.876731
23	H	5.852618	4.669195	6.127724	5.333607	5.948324
24	C	5.087415	4.257758	4.866484	3.771666	4.111087
25	H	6.141681	5.344170	5.825983	4.659480	4.819801
26	C	4.258972	3.741850	3.743485	2.517920	2.733768
27	H	4.884927	4.600024	4.080194	2.757481	2.524060
28	C	3.082707	3.028864	3.478527	3.718860	4.431475
29	C	3.551268	3.917410	2.957793	2.774547	2.929466
30	O	3.388631	3.818274	3.282183	3.589015	4.015499
31	O	4.419411	4.961510	3.531756	3.292561	3.041601
32	O	3.661121	3.544312	4.363730	4.792248	5.572470
33	C	2.479538	1.434929	3.746911	4.138888	5.225493
34	N	3.536913	2.598555	4.867282	5.299952	6.385306

		6	7	8	9	10
6	C	0.000000				
7	H	1.083832	0.000000			
8	C	1.414699	2.206808	0.000000		

This journal is © The Royal Society of Chemistry 2014

9	H	2.234121	2.661154	1.080985	0.000000	
10	C	4.326961	5.307407	3.895766	4.549661	0.000000
11	H	4.979805	5.967460	4.265520	4.729334	1.086008
12	C	4.982073	5.957000	4.833621	5.645312	1.384742
13	H	5.981502	6.984723	5.734619	6.510384	2.141052
14	C	4.728962	5.590929	4.987118	5.927626	2.428938
15	H	5.607177	6.428547	5.961831	6.938753	3.407226
16	C	3.707516	4.432912	4.256343	5.210115	2.816671
17	H	3.992123	4.524408	4.832417	5.807527	3.903065
18	C	2.654950	2.714066	3.067115	3.340884	4.262135
19	C	3.089945	3.406604	2.814429	2.804760	3.778629
20	C	4.210678	4.317974	3.778791	3.375119	4.912197
21	H	4.884911	5.108648	4.166266	3.615746	5.043368
22	C	4.833292	4.636479	4.693551	4.263156	6.114942
23	H	5.828475	5.590760	5.588710	5.021632	7.007124
24	C	4.571070	4.159468	4.850327	4.633439	6.424307
25	H	5.442256	4.883713	5.820408	5.571015	7.479585
26	C	3.571107	3.197451	4.147751	4.231761	5.639707
27	H	3.874262	3.338704	4.744728	4.960126	6.245438
28	C	2.332820	3.299625	1.474685	2.221663	3.585319
29	C	1.494994	2.216936	2.327887	3.332078	4.361040
30	O	2.334499	3.282080	2.331049	3.314212	3.820655
31	O	2.441889	2.805502	3.501825	4.470805	5.159155
32	O	3.511139	4.442609	2.438753	2.827381	3.793835
33	C	4.126692	4.861179	3.061204	2.936978	2.928972
34	N	5.141589	5.862816	3.935397	3.630558	3.672335

		11	12	13	14	15
11	H	0.000000				
12	C	2.150948	0.000000			
13	H	2.473841	1.086329	0.000000		
14	C	3.416436	1.410524	2.165390	0.000000	
15	H	4.306842	2.165864	2.488329	1.086314	0.000000
16	C	3.902536	2.425429	3.404612	1.385279	2.144506
17	H	4.988788	3.415052	4.307190	2.152799	2.480643
18	C	4.902319	5.069837	6.126608	4.862532	5.822323
19	C	4.131051	4.885812	5.849552	5.080647	6.135089
20	C	5.047372	6.109328	7.003560	6.416359	7.471913
21	H	4.942024	6.341897	7.128822	6.865063	7.937528
22	C	6.351240	7.214446	8.156859	7.338110	8.348840
23	H	7.136458	8.154697	9.056344	8.353110	9.369556
24	C	6.875968	7.340558	8.357468	7.190682	8.123996
25	H	7.948529	8.350649	9.373307	8.123153	9.013356
26	C	6.265656	6.396649	7.455448	6.068760	6.954752
27	H	6.986976	6.822120	7.896046	6.275913	7.051377
28	C	3.870196	4.341084	5.073871	4.633392	5.511048
29	C	5.107613	4.654949	5.560483	4.228023	4.922235
30	O	4.385831	4.142357	4.888050	4.061976	4.767610
31	O	6.009689	5.180111	6.051486	4.457660	4.933285
32	O	3.764712	4.592215	5.117146	5.170562	6.012158
33	C	2.604963	4.311908	4.965785	5.142242	6.205263
34	N	3.028997	5.029879	5.499730	6.034634	7.060929

		16	17	18	19	20

This journal is © The Royal Society of Chemistry 2014

16	C	0.000000				
17	H	1.086633	0.000000			
18	C	3.743056	4.080688	0.000000		
19	C	4.255807	4.882100	1.418431	0.000000	
20	C	5.635765	6.242556	2.445949	1.412206	0.000000
21	H	6.259820	6.982280	3.430126	2.167017	1.086257
22	C	6.398101	6.825467	2.802937	2.422036	1.386155
23	H	7.455696	7.898781	3.889303	3.406614	2.143014
24	C	6.072259	6.281735	2.422555	2.806952	2.428524
25	H	6.957556	7.057042	3.408281	3.893361	3.407912
26	C	4.857693	4.969375	1.409343	2.444759	2.812596
27	H	4.967079	4.838030	2.162055	3.427825	3.900054
28	C	4.245371	4.907614	4.269457	3.961167	4.999509
29	C	3.373184	3.536912	3.849713	4.328008	5.570843
30	O	3.635148	4.091555	4.558304	4.645524	5.867303
31	O	3.556118	3.365439	4.526567	5.254551	6.518039
32	O	5.059310	5.828026	5.230850	4.670125	5.557739
33	C	4.920543	5.869698	3.741227	2.471769	2.913816
34	N	5.970021	6.956480	4.845829	3.508462	3.615951

		21	22	23	24	25
21	H	0.000000				
22	C	2.150381	0.000000			
23	H	2.473172	1.086440	0.000000		
24	C	3.415248	1.410149	2.165726	0.000000	
25	H	4.306642	2.166283	2.489914	1.086506	0.000000
26	C	3.898828	2.424663	3.404980	1.386704	2.146864
27	H	4.986266	3.414467	4.307764	2.153061	2.481287
28	C	5.222477	6.053599	6.936732	6.260138	7.253250
29	C	6.185012	6.269505	7.286584	5.953015	6.801802
30	O	6.266486	6.801266	7.775194	6.743919	7.686484
31	O	7.222478	7.080596	8.118540	6.563282	7.310834
32	O	5.555086	6.728332	7.521286	7.128211	8.145804
33	C	2.588075	4.298017	4.949461	5.131117	6.194042
34	N	2.960567	4.969486	5.429042	5.984803	7.007969

		26	27	28	29	30
26	C	0.000000				
27	H	1.087495	0.000000			
28	C	5.476615	6.007509	0.000000		
29	C	4.821412	4.939964	2.281429	0.000000	
30	O	5.726655	6.027046	1.411226	1.385140	0.000000
31	O	5.322602	5.198279	3.423233	1.203022	2.269727
32	O	6.469899	7.089285	1.200926	3.410425	2.277220
33	C	4.910443	5.862852	3.428427	4.946929	4.527574
34	N	5.933978	6.927430	4.118473	5.914942	5.334260

		31	32	33	34	
31	O	0.000000				
32	O	4.484211	0.000000			
33	C	6.077155	3.465966	0.000000		
34	N	7.074869	3.835059	1.163773	0.000000	

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96

This journal is © The Royal Society of Chemistry 2014

```
 Full point group                 C1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6              0       -0.530896    0.775196    0.982851
    2          6              0        0.599285    1.172825    0.166371
    3          6              0       -0.651319   -0.614686    1.251656
    4          6              0        0.331341   -1.482634    0.639703
    5          1              0        0.207367   -2.552382    0.800311
    6          6              0       -0.160234   -1.338562   -1.350058
    7          1              0        0.540555   -2.102515   -1.666227
    8          6              0       -0.089227    0.009873   -1.772022
    9          1              0        0.717820    0.469718   -2.324964
   10          6              0       -1.523164    1.666070    1.449442
   11          1              0       -1.443850    2.725727    1.225276
   12          6              0       -2.581431    1.182321    2.200154
   13          1              0       -3.332559    1.871556    2.575482
   14          6              0       -2.699378   -0.196629    2.472482
   15          1              0       -3.540135   -0.561121    3.055879
   16          6              0       -1.757996   -1.088996    1.986189
   17          1              0       -1.859277   -2.155358    2.168910
   18          6              0        1.686043   -0.981690    0.524153
   19          6              0        1.829536    0.402416    0.249183
   20          6              0        3.114658    0.934706    0.005354
   21          1              0        3.226941    1.992748   -0.213493
   22          6              0        4.227101    0.110164    0.068814
   23          1              0        5.216443    0.528418   -0.094330
   24          6              0        4.085066   -1.265740    0.343107
   25          1              0        4.965335   -1.900837    0.390786
   26          6              0        2.826354   -1.809491    0.550291
   27          1              0        2.710644   -2.871917    0.751557
   28          6              0       -1.470091    0.499350   -1.940316
   29          6              0       -1.612190   -1.694075   -1.329077
   30          8              0       -2.344249   -0.540942   -1.559265
   31          8              0       -2.133709   -2.759819   -1.130406
   32          8              0       -1.892687    1.555690   -2.324740
   33          6              0        0.698407    2.543767   -0.245593
   34          7              0        0.803526    3.653062   -0.581426
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3914929      0.2664849
0.2437577


*********************************************************************

            Population analysis using the SCF density.
```

This journal is © The Royal Society of Chemistry 2014

```
**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.22845 -19.17634 -19.17307 -14.36621 -
10.34996
 Alpha  occ. eigenvalues --  -10.34542 -10.28700 -10.26152 -10.25490 -
10.25392
 Alpha  occ. eigenvalues --  -10.24860 -10.24700 -10.24396 -10.24232 -
10.23844
 Alpha  occ. eigenvalues --  -10.23140 -10.23033 -10.22970 -10.22893 -
10.22416
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha  occ. eigenvalues --  -10.22318 -10.22270 -10.22215  -1.14736
-1.08340
 Alpha  occ. eigenvalues --   -1.04510  -0.94199  -0.92249  -0.88957
-0.85255
 Alpha  occ. eigenvalues --   -0.83835  -0.82512  -0.78681  -0.77969
-0.74994
 Alpha  occ. eigenvalues --   -0.71077  -0.69483  -0.66427  -0.64973
-0.63916
 Alpha  occ. eigenvalues --   -0.63110  -0.59465  -0.58700  -0.56010
-0.55767
 Alpha  occ. eigenvalues --   -0.51998  -0.51528  -0.50610  -0.50163
-0.49574
 Alpha  occ. eigenvalues --   -0.48523  -0.48082  -0.46502  -0.46257
-0.45964
 Alpha  occ. eigenvalues --   -0.45181  -0.44775  -0.44661  -0.43343
-0.42533
 Alpha  occ. eigenvalues --   -0.41253  -0.41012  -0.39513  -0.39023
-0.38406
 Alpha  occ. eigenvalues --   -0.38330  -0.37868  -0.36924  -0.36324
-0.35432
 Alpha  occ. eigenvalues --   -0.33948  -0.32435  -0.32136  -0.29681
-0.28778
 Alpha  occ. eigenvalues --   -0.28124  -0.27820  -0.25075
 Alpha virt. eigenvalues --   -0.12231  -0.08477  -0.04705  -0.04035
-0.03502
 Alpha virt. eigenvalues --   -0.01530  -0.01247  -0.00121   0.00229
0.00623
 Alpha virt. eigenvalues --    0.00641   0.01957   0.02003   0.02313
0.03043
 Alpha virt. eigenvalues --    0.03470   0.03534   0.04203   0.04526
0.05783
 Alpha virt. eigenvalues --    0.05897   0.06297   0.06376   0.06511
0.06774
 Alpha virt. eigenvalues --    0.07374   0.08057   0.08142   0.08733
0.09627
 Alpha virt. eigenvalues --    0.09893   0.10232   0.10368   0.10790
0.11082
 Alpha virt. eigenvalues --    0.11282   0.11773   0.12110   0.12435
0.13096
 Alpha virt. eigenvalues --    0.13553   0.13729   0.14072   0.14225
0.14529
 Alpha virt. eigenvalues --    0.14832   0.15497   0.15614   0.16039
0.16359
 Alpha virt. eigenvalues --    0.16511   0.16844   0.17188   0.17354
0.17988
 Alpha virt. eigenvalues --    0.18216   0.18516   0.18633   0.19025
0.19212
 Alpha virt. eigenvalues --    0.19668   0.19887   0.20244   0.20338
0.20701
 Alpha virt. eigenvalues --    0.21086   0.21914   0.22048   0.22346
0.22551
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.22752   0.22830   0.23228   0.23621
0.24023
 Alpha virt. eigenvalues --    0.24237   0.24536   0.24853   0.25619
0.25994
 Alpha virt. eigenvalues --    0.26044   0.26282   0.26384   0.26735
0.27233
 Alpha virt. eigenvalues --    0.27300   0.27511   0.27847   0.28165
0.28456
 Alpha virt. eigenvalues --    0.28605   0.28677   0.29213   0.29228
0.29543
 Alpha virt. eigenvalues --    0.29933   0.30280   0.30813   0.31086
0.32538
 Alpha virt. eigenvalues --    0.33462   0.33859   0.34072   0.34186
0.34659
 Alpha virt. eigenvalues --    0.34847   0.35287   0.35693   0.35780
0.36105
 Alpha virt. eigenvalues --    0.36613   0.37072   0.37510   0.38730
0.39021
 Alpha virt. eigenvalues --    0.39974   0.40402   0.40617   0.41798
0.42832
 Alpha virt. eigenvalues --    0.43139   0.43662   0.44124   0.44677
0.45115
 Alpha virt. eigenvalues --    0.46189   0.47503   0.51233   0.51979
0.55300
 Alpha virt. eigenvalues --    0.56638   0.57043   0.59215   0.61542
0.62660
 Alpha virt. eigenvalues --    0.65191   0.66155   0.67821   0.68385
0.68892
 Alpha virt. eigenvalues --    0.69302   0.70633   0.71280   0.71675
0.72259
 Alpha virt. eigenvalues --    0.72403   0.73518   0.73828   0.74347
0.75093
 Alpha virt. eigenvalues --    0.75167   0.75565   0.76402   0.77351
0.78188
 Alpha virt. eigenvalues --    0.79564   0.79675   0.80354   0.80919
0.81217
 Alpha virt. eigenvalues --    0.82346   0.82971   0.83415   0.84820
0.86310
 Alpha virt. eigenvalues --    0.86452   0.87733   0.88223   0.88666
0.89786
 Alpha virt. eigenvalues --    0.90227   0.90707   0.91924   0.92443
0.92638
 Alpha virt. eigenvalues --    0.93102   0.93789   0.94778   0.95073
0.95770
 Alpha virt. eigenvalues --    0.96718   0.97665   0.99345   1.00516
1.01466
 Alpha virt. eigenvalues --    1.02636   1.03416   1.04813   1.05324
1.06219
 Alpha virt. eigenvalues --    1.06887   1.07785   1.08567   1.10239
1.10522
 Alpha virt. eigenvalues --    1.11484   1.12810   1.13353   1.15500
1.15978
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    1.17075   1.18459   1.19500   1.20110
1.20475
 Alpha virt. eigenvalues --    1.21736   1.22870   1.24377   1.25075
1.25713
 Alpha virt. eigenvalues --    1.26890   1.27542   1.27971   1.28773
1.30343
 Alpha virt. eigenvalues --    1.31652   1.32647   1.33040   1.34858
1.36107
 Alpha virt. eigenvalues --    1.36494   1.37933   1.38134   1.39337
1.40536
 Alpha virt. eigenvalues --    1.41357   1.42150   1.42438   1.43192
1.43549
 Alpha virt. eigenvalues --    1.44695   1.45010   1.46134   1.46494
1.46939
 Alpha virt. eigenvalues --    1.47193   1.48828   1.49329   1.50413
1.51208
 Alpha virt. eigenvalues --    1.52996   1.53803   1.56047   1.56825
1.58802
 Alpha virt. eigenvalues --    1.62111   1.64388   1.66470   1.67044
1.69243
 Alpha virt. eigenvalues --    1.72098   1.72639   1.75637   1.77304
1.78637
 Alpha virt. eigenvalues --    1.79648   1.80543   1.81540   1.82276
1.82682
 Alpha virt. eigenvalues --    1.83537   1.84829   1.86404   1.87155
1.87601
 Alpha virt. eigenvalues --    1.88044   1.89238   1.91279   1.91675
1.92394
 Alpha virt. eigenvalues --    1.92887   1.93644   1.94645   1.95048
1.96932
 Alpha virt. eigenvalues --    1.97513   1.98165   1.98884   1.99812
2.01894
 Alpha virt. eigenvalues --    2.02365   2.03945   2.05552   2.06649
2.07152
 Alpha virt. eigenvalues --    2.08682   2.09882   2.11809   2.12371
2.13087
 Alpha virt. eigenvalues --    2.14945   2.17754   2.18667   2.18975
2.20171
 Alpha virt. eigenvalues --    2.21868   2.23800   2.24793   2.25336
2.26709
 Alpha virt. eigenvalues --    2.27572   2.28759   2.29836   2.30371
2.31564
 Alpha virt. eigenvalues --    2.32249   2.32655   2.35462   2.37709
2.39411
 Alpha virt. eigenvalues --    2.41369   2.42110   2.47215   2.48296
2.49227
 Alpha virt. eigenvalues --    2.55194   2.59083   2.59583   2.60099
2.61447
 Alpha virt. eigenvalues --    2.62425   2.64796   2.65959   2.67796
2.69154
 Alpha virt. eigenvalues --    2.70355   2.71837   2.73617   2.75072
2.75970
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    2.77145   2.81640   2.82552   2.83599
2.84920
 Alpha virt. eigenvalues --    2.85635   2.86329   2.88987   2.92588
2.94639
 Alpha virt. eigenvalues --    2.96485   2.97688   3.08564   3.10952
3.15261
 Alpha virt. eigenvalues --    3.17027   3.18426   3.23304   3.24523
3.33072
 Alpha virt. eigenvalues --    3.33683   3.41095   3.47380   4.23913
4.28601
 Alpha virt. eigenvalues --    4.31277   4.32270   4.33836   4.35584
4.37012
 Alpha virt. eigenvalues --    4.38854   4.42722   4.45122   4.46280
4.47268
 Alpha virt. eigenvalues --    4.49573   4.51511   4.52672   4.61350
4.62883
 Alpha virt. eigenvalues --    4.68589   4.71857   4.74052   4.85072
4.99943
 Alpha virt. eigenvalues --    5.29805
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   46.338141 -15.713238  10.846990 -19.100690   0.037658
0.612542
     2  C  -15.713238  28.304933  -9.055809  16.678637  -0.014514  -
1.455960
     3  C   10.846990  -9.055809  23.325615 -15.871233  -0.018324
1.046404
     4  C  -19.100690  16.678637 -15.871233  39.596828   0.213030  -
1.235378
     5  H    0.037658  -0.014514  -0.018324   0.213030   0.518879  -
0.000975
     6  C    0.612542  -1.455960   1.046404  -1.235378  -0.000975
9.334060
     7  H    0.022610   0.004006   0.003533  -0.055299  -0.002105
0.351589
     8  C   -0.302125   0.168158   0.072146  -0.711017   0.017639  -
1.879739
     9  H   -0.001416   0.004528   0.018613  -0.006838  -0.000046  -
0.010396
    10  C  -19.452219   5.137765  -3.643203   5.217475  -0.002875
0.147708
    11  H   -0.105548  -0.030278   0.062420   0.008688   0.000002
0.002999
    12  C    0.464290  -0.906923   1.213624  -0.499301   0.004466  -
0.135262
    13  H    0.009956  -0.016888   0.021045   0.003700   0.000000
0.001534
    14  C   -1.843824   0.723730  -2.483555   0.632405   0.009855
0.149306
    15  H    0.025160   0.008882   0.016744  -0.013590  -0.000007  -
0.002396
```

This journal is © The Royal Society of Chemistry 2014

16	C	-6.243421	1.148456	-5.062719	4.585785	0.026138	0.283109
17	H	0.074496	0.018403	-0.045560	-0.037786	0.003849	-0.010971
18	C	7.017015	-8.093422	6.070390	-13.352276	-0.022417	0.225786
19	C	8.360550	-11.363404	5.424234	-15.281614	0.017385	1.055683
20	C	-0.406059	1.443313	-1.228054	1.380970	0.008547	-0.442481
21	H	0.014280	-0.018815	-0.001419	-0.002751	0.000002	-0.001913
22	C	-0.023879	-0.614982	0.143185	-0.131289	-0.000632	-0.017772
23	H	-0.001954	-0.005465	0.000906	0.002479	0.000000	0.000011
24	C	-0.163027	0.467602	-0.461255	0.212304	-0.004841	-0.005733
25	H	0.000546	0.006620	-0.002794	-0.001249	-0.000006	-0.000428
26	C	-0.782081	-1.338453	0.405680	0.444799	0.003848	-0.044487
27	H	-0.000049	0.005525	-0.008584	-0.026890	0.003609	0.002818
28	C	-0.173502	0.594000	-0.454032	0.677943	-0.001983	0.741720
29	C	-0.821217	1.055453	-0.855009	1.638192	-0.026815	-1.590831
30	O	-0.045664	0.057705	-0.127325	0.111847	0.000246	-0.390332
31	O	0.063724	-0.059904	0.150436	-0.180370	0.005430	-0.050397
32	O	0.239965	-0.114749	0.027368	-0.077591	0.000036	-0.050065
33	C	-3.230771	-1.281771	-3.296964	0.542679	0.004352	-0.487046
34	N	-0.089955	0.218917	0.144562	0.025550	-0.000002	0.024128

		7	8	9	10	11	12
1	C	0.022610	-0.302125	-0.001416	-19.452219	-0.105548	0.464290
2	C	0.004006	0.168158	0.004528	5.137765	-0.030278	-0.906923
3	C	0.003533	0.072146	0.018613	-3.643203	0.062420	1.213624
4	C	-0.055299	-0.711017	-0.006838	5.217475	0.008688	-0.499301
5	H	-0.002105	0.017639	-0.000046	-0.002875	0.000002	0.004466
6	C	0.351589	-1.879739	-0.010396	0.147708	0.002999	-0.135262

This journal is © The Royal Society of Chemistry 2014

7	H	0.468710	-0.001487	-0.001893	-0.001579	0.000000	0.000574
8	C	-0.001487	8.929580	0.347812	0.538074	-0.009199	0.191305
9	H	-0.001893	0.347812	0.458711	0.007324	-0.000001	-0.000974
10	C	-0.001579	0.538074	0.007324	21.810742	0.296411	-2.066724
11	H	0.000000	-0.009199	-0.000001	0.296411	0.501538	0.119306
12	C	0.000574	0.191305	-0.000974	-2.066724	0.119306	8.694373
13	H	0.000000	-0.001857	0.000000	0.023119	-0.003981	0.287580
14	C	-0.000249	-0.027843	0.000631	0.884209	0.009586	0.630511
15	H	0.000000	0.001049	0.000000	0.021519	-0.000151	-0.044807
16	C	0.007673	0.179073	-0.003690	4.560180	-0.011756	-1.220009
17	H	0.000000	0.004965	0.000000	-0.022695	0.000015	0.001569
18	C	0.030248	0.020542	0.005085	-3.421857	-0.002240	-0.038026
19	C	0.015715	-0.395638	0.060444	-2.348338	-0.011802	-0.038027
20	C	-0.002801	-0.027420	-0.042164	-1.506723	-0.003950	-0.043763
21	H	0.000001	0.001175	-0.000050	-0.003981	0.000000	0.000147
22	C	0.003915	0.063199	-0.007578	0.172835	-0.000456	-0.019390
23	H	0.000000	-0.000024	0.000000	0.000135	0.000000	0.000002
24	C	-0.012485	-0.107057	-0.003843	-0.165798	-0.000038	-0.010240
25	H	0.000002	0.000081	0.000000	-0.000092	0.000000	0.000008
26	C	-0.034332	-0.112134	0.002084	-0.569236	-0.000215	-0.021640
27	H	-0.000027	-0.000799	0.000000	0.000313	0.000000	-0.000153
28	C	0.008629	-1.577004	-0.072824	-0.274180	0.009077	-0.145334
29	C	-0.075376	0.810530	0.014161	0.132171	-0.001953	0.107987
30	O	0.007607	-0.221690	0.008380	-0.003761	0.000044	0.011223
31	O	0.001144	-0.063943	-0.000547	-0.024754	-0.000002	-0.004122
32	O	-0.000530	-0.110387	0.002481	-0.120428	0.000142	-0.015001

This journal is © The Royal Society of Chemistry 2014

```
    33  C    0.006241   0.068144  -0.032648   1.104302  -0.056128  -
0.130427
    34  N   -0.000128   0.005356   0.000666   0.088459   0.010920
0.038434
             13         14         15         16         17         18
     1  C    0.009956  -1.843824   0.025160  -6.243421   0.074496
7.017015
     2  C   -0.016888   0.723730   0.008882   1.148456   0.018403  -
8.093422
     3  C    0.021045  -2.483555   0.016744  -5.062719  -0.045560
6.070390
     4  C    0.003700   0.632405  -0.013590   4.585785  -0.037786 -
13.352276
     5  H    0.000000   0.009855  -0.000007   0.026138   0.003849  -
0.022417
     6  C    0.001534   0.149306  -0.002396   0.283109  -0.010971
0.225786
     7  H    0.000000  -0.000249   0.000000   0.007673   0.000000
0.030248
     8  C   -0.001857  -0.027843   0.001049   0.179073   0.004965
0.020542
     9  H    0.000000   0.000631   0.000000  -0.003690   0.000000
0.005085
    10  C    0.023119   0.884209   0.021519   4.560180  -0.022695  -
3.421857
    11  H   -0.003981   0.009586  -0.000151  -0.011756   0.000015  -
0.002240
    12  C    0.287580   0.630511  -0.044807  -1.220009   0.001569  -
0.038026
    13  H    0.515199  -0.046341  -0.004161   0.019428  -0.000157
0.002556
    14  C   -0.046341   7.747403   0.294773   1.169792   0.071982  -
0.875461
    15  H   -0.004161   0.294773   0.517908  -0.012954  -0.004284  -
0.002574
    16  C    0.019428   1.169792  -0.012954  11.137838   0.262953  -
1.654177
    17  H   -0.000157   0.071982  -0.004284   0.262953   0.524967  -
0.043044
    18  C    0.002556  -0.875461  -0.002574  -1.654177  -0.043044
19.823643
    19  C   -0.002110  -0.363639   0.001628  -1.809399  -0.005363
6.948774
    20  C    0.000091  -0.119126  -0.000172  -0.460807   0.000207
0.014853
    21  H    0.000000  -0.000082   0.000000  -0.000025   0.000000
0.032810
    22  C   -0.000003   0.013463   0.000018   0.075825  -0.000096
0.316636
    23  H    0.000000   0.000004   0.000000  -0.000088   0.000000
0.008174
```

This journal is © The Royal Society of Chemistry 2014

24	C	0.000016	-0.022771	-0.000006	-0.126531	-0.000260	-1.401620
25	H	0.000000	-0.000002	0.000000	0.000233	0.000000	0.021415
26	C	-0.000087	-0.111217	0.000210	-0.696217	0.001083	-1.254816
27	H	0.000000	0.000686	0.000000	0.003165	0.000002	-0.038327
28	C	0.003033	-0.008283	-0.001462	-0.056116	-0.003135	-0.106389
29	C	-0.001950	-0.074750	0.003675	-0.052744	0.010276	-0.616069
30	O	-0.000020	0.025822	-0.000040	-0.011721	0.000309	-0.041431
31	O	0.000001	-0.039163	-0.000091	-0.077811	-0.000136	0.094386
32	O	-0.000078	-0.006341	0.000001	-0.003864	-0.000001	0.030782
33	C	-0.004633	-0.050170	0.001332	-0.119423	0.001039	-3.433500
34	N	0.000036	0.009368	-0.000007	0.016553	0.000002	0.108979

		19	20	21	22	23	24
1	C	8.360550	-0.406059	0.014280	-0.023879	-0.001954	-0.163027
2	C	-11.363404	1.443313	-0.018815	-0.614982	-0.005465	0.467602
3	C	5.424234	-1.228054	-0.001419	0.143185	0.000906	-0.461255
4	C	-15.281614	1.380970	-0.002751	-0.131289	0.002479	0.212304
5	H	0.017385	0.008547	0.000002	-0.000632	0.000000	-0.004841
6	C	1.055683	-0.442481	-0.001913	-0.017772	0.000011	-0.005733
7	H	0.015715	-0.002801	0.000001	0.003915	0.000000	-0.012485
8	C	-0.395638	-0.027420	0.001175	0.063199	-0.000024	-0.107057
9	H	0.060444	-0.042164	-0.000050	-0.007578	0.000000	-0.003843
10	C	-2.348338	-1.506723	-0.003981	0.172835	0.000135	-0.165798
11	H	-0.011802	-0.003950	0.000000	-0.000456	0.000000	-0.000038
12	C	-0.038027	-0.043763	0.000147	-0.019390	0.000002	-0.010240
13	H	-0.002110	0.000091	0.000000	-0.000003	0.000000	0.000016
14	C	-0.363639	-0.119126	-0.000082	0.013463	0.000004	-0.022771

This journal is © The Royal Society of Chemistry 2014

15	H	0.001628	-0.000172	0.000000	0.000018	0.000000	-0.000006
16	C	-1.809399	-0.460807	-0.000025	0.075825	-0.000088	-0.126531
17	H	-0.005363	0.000207	0.000000	-0.000096	0.000000	-0.000260
18	C	6.948774	0.014853	0.032810	0.316636	0.008174	-1.401620
19	C	33.237443	-12.416778	-0.111087	2.170664	0.004096	-1.158220
20	C	-12.416778	18.985543	0.313583	-3.161916	0.013309	0.649562
21	H	-0.111087	0.313583	0.497737	0.074988	-0.003985	0.021299
22	C	2.170664	-3.161916	0.074988	7.554121	0.306292	0.404261
23	H	0.004096	0.013309	-0.003985	0.306292	0.515163	-0.035532
24	C	-1.158220	0.649562	0.021299	0.404261	-0.035532	7.417369
25	H	0.002036	0.012136	-0.000148	-0.034984	-0.004067	0.306482
26	C	-2.635649	2.833185	-0.012730	-1.051368	0.010465	0.366337
27	H	0.073278	-0.030531	0.000016	0.004830	-0.000154	0.016069
28	C	-0.225701	0.233709	0.002379	0.044407	0.000085	0.009379
29	C	-0.671361	-0.010705	-0.000701	-0.029855	-0.000066	0.110493
30	O	-0.040346	0.021189	0.000001	-0.002704	0.000000	0.002813
31	O	0.037736	0.002531	0.000000	-0.000008	0.000000	-0.000840
32	O	0.006631	0.002863	-0.000012	-0.002946	0.000000	0.000293
33	C	-2.730090	0.260979	-0.024240	0.162481	-0.004400	-0.131064
34	N	-0.010876	-0.028120	0.006571	0.007219	0.000088	0.001703

		25	26	27	28	29	30
1	C	0.000546	-0.782081	-0.000049	-0.173502	-0.821217	-0.045664
2	C	0.006620	-1.338453	0.005525	0.594000	1.055453	0.057705
3	C	-0.002794	0.405680	-0.008584	-0.454032	-0.855009	-0.127325
4	C	-0.001249	0.444799	-0.026890	0.677943	1.638192	0.111847
5	H	-0.000006	0.003848	0.003609	-0.001983	-0.026815	0.000246

This journal is © The Royal Society of Chemistry 2014

```
     6  C   -0.000428  -0.044487   0.002818   0.741720  -1.590831  -
0.390332
     7  H    0.000002  -0.034332  -0.000027   0.008629  -0.075376
0.007607
     8  C    0.000081  -0.112134  -0.000799  -1.577004   0.810530  -
0.221690
     9  H    0.000000   0.002084   0.000000  -0.072824   0.014161
0.008380
    10  C   -0.000092  -0.569236   0.000313  -0.274180   0.132171  -
0.003761
    11  H    0.000000  -0.000215   0.000000   0.009077  -0.001953
0.000044
    12  C    0.000008  -0.021640  -0.000153  -0.145334   0.107987
0.011223
    13  H    0.000000  -0.000087   0.000000   0.003033  -0.001950  -
0.000020
    14  C   -0.000002  -0.111217   0.000686  -0.008283  -0.074750
0.025822
    15  H    0.000000   0.000210   0.000000  -0.001462   0.003675  -
0.000040
    16  C    0.000233  -0.696217   0.003165  -0.056116  -0.052744  -
0.011721
    17  H    0.000000   0.001083   0.000002  -0.003135   0.010276
0.000309
    18  C    0.021415  -1.254816  -0.038327  -0.106389  -0.616069  -
0.041431
    19  C    0.002036  -2.635649   0.073278  -0.225701  -0.671361  -
0.040346
    20  C    0.012136   2.833185  -0.030531   0.233709  -0.010705
0.021189
    21  H   -0.000148  -0.012730   0.000016   0.002379  -0.000701
0.000001
    22  C   -0.034984  -1.051368   0.004830   0.044407  -0.029855  -
0.002704
    23  H   -0.004067   0.010465  -0.000154   0.000085  -0.000066
0.000000
    24  C    0.306482   0.366337   0.016069   0.009379   0.110493
0.002813
    25  H    0.518011  -0.013305  -0.004257  -0.000064   0.000127
0.000000
    26  C   -0.013305  10.436877   0.276938   0.026071  -0.046654
0.022828
    27  H   -0.004257   0.276938   0.528847  -0.000821   0.003347
0.000004
    28  C   -0.000064   0.026071  -0.000821   6.714544  -0.942741
0.274327
    29  C    0.000127  -0.046654   0.003347  -0.942741   6.822169
0.325923
    30  O    0.000000   0.022828   0.000004   0.274327   0.325923
8.311678
    31  O    0.000000   0.018918   0.000004   0.042566   0.413367  -
0.086803
```

```
    32  O    0.000000   0.001420   0.000000   0.495114   0.013290  -
0.069001
    33  C    0.000714  -0.356788   0.001411   0.082104   0.133424
0.052490
    34  N    0.000000   0.006826  -0.000002  -0.029473  -0.003202  -
0.001229
              31         32         33         34
     1  C    0.063724   0.239965  -3.230771  -0.089955
     2  C   -0.059904  -0.114749  -1.281771   0.218917
     3  C    0.150436   0.027368  -3.296964   0.144562
     4  C   -0.180370  -0.077591   0.542679   0.025550
     5  H    0.005430   0.000036   0.004352  -0.000002
     6  C   -0.050397  -0.050065  -0.487046   0.024128
     7  H    0.001144  -0.000530   0.006241  -0.000128
     8  C   -0.063943  -0.110387   0.068144   0.005356
     9  H   -0.000547   0.002481  -0.032648   0.000666
    10  C   -0.024754  -0.120428   1.104302   0.088459
    11  H   -0.000002   0.000142  -0.056128   0.010920
    12  C   -0.004122  -0.015001  -0.130427   0.038434
    13  H    0.000001  -0.000078  -0.004633   0.000036
    14  C   -0.039163  -0.006341  -0.050170   0.009368
    15  H   -0.000091   0.000001   0.001332  -0.000007
    16  C   -0.077811  -0.003864  -0.119423   0.016553
    17  H   -0.000136  -0.000001   0.001039   0.000002
    18  C    0.094386   0.030782  -3.433500   0.108979
    19  C    0.037736   0.006631  -2.730090  -0.010876
    20  C    0.002531   0.002863   0.260979  -0.028120
    21  H    0.000000  -0.000012  -0.024240   0.006571
    22  C   -0.000008  -0.002946   0.162481   0.007219
    23  H    0.000000   0.000000  -0.004400   0.000088
    24  C   -0.000840   0.000293  -0.131064   0.001703
    25  H    0.000000   0.000000   0.000714   0.000000
    26  C    0.018918   0.001420  -0.356788   0.006826
    27  H    0.000004   0.000000   0.001411  -0.000002
    28  C    0.042566   0.495114   0.082104  -0.029473
    29  C    0.413367   0.013290   0.133424  -0.003202
    30  O   -0.086803  -0.069001   0.052490  -0.001229
    31  O    8.140566   0.000107  -0.000967  -0.000002
    32  O    0.000107   8.089810   0.014164  -0.001287
    33  C   -0.000967   0.014164  19.290639  -0.261092
    34  N   -0.000002  -0.001287  -0.261092   7.089360
 Mulliken atomic charges:
              1
     1  C    0.372714
     2  C    0.037942
     3  C   -0.378055
     4  C    0.611853
     5  H    0.220571
     6  C   -0.166835
     7  H    0.256091
     8  C    0.130533
     9  H    0.253987
```

This journal is © The Royal Society of Chemistry 2014

```
    10  C   -0.514300
    11  H    0.216548
    12  C   -0.425274
    13  H    0.194970
    14  C   -0.300710
    15  H    0.193803
    16  C    0.147274
    17  H    0.197373
    18  C   -0.374429
    19  C    0.203147
    20  C   -0.245001
    21  H    0.216949
    22  C   -0.418483
    23  H    0.194528
    24  C   -0.174820
    25  H    0.192985
    26  C    0.223839
    27  H    0.189734
    28  C    0.113958
    29  C    0.227415
    30  O   -0.192368
    31  O   -0.381055
    32  O   -0.352183
    33  C   -0.094375
    34  N   -0.378325
Sum of Mulliken charges=   0.00000
Atomic charges with hydrogens summed into heavy atoms:
             1
     1  C    0.372714
     2  C    0.037942
     3  C   -0.378055
     4  C    0.832424
     5  H    0.000000
     6  C    0.089256
     7  H    0.000000
     8  C    0.384520
     9  H    0.000000
    10  C   -0.297752
    11  H    0.000000
    12  C   -0.230304
    13  H    0.000000
    14  C   -0.106907
    15  H    0.000000
    16  C    0.344648
    17  H    0.000000
    18  C   -0.374429
    19  C    0.203147
    20  C   -0.028052
    21  H    0.000000
    22  C   -0.223956
    23  H    0.000000
    24  C    0.018165
```

```
    25  H    0.000000
    26  C    0.413573
    27  H    0.000000
    28  C    0.113958
    29  C    0.227415
    30  O   -0.192368
    31  O   -0.381055
    32  O   -0.352183
    33  C   -0.094375
    34  N   -0.378325
 Sum of Mulliken charges=   0.00000
 Electronic spatial extent (au):  <R**2>=  5307.7528
 Charge=     0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=     4.7062    Y=    -3.6140    Z=     3.3804  Tot=     6.8291
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=  -125.1407   YY=  -146.9616   ZZ=  -132.7646
   XY=    -9.2629   XZ=   -14.6688   YZ=     4.1209
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=     9.8150   YY=   -12.0060   ZZ=     2.1910
   XY=    -9.2629   XZ=   -14.6688   YZ=     4.1209
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=    55.3576  YYY=   -65.8993  ZZZ=   -20.8836  XYY=    13.7673
  XXY=     6.1522  XXZ=    36.3188  XZZ=   -18.7665  YZZ=   -18.1326
  YYZ=    36.5110  XYZ=    -5.3560
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX= -3333.6489 YYYY= -2364.2125 ZZZZ= -1607.3896 XXXY=   -59.5661
 XXXZ=  -110.8967 YYYX=  -150.2121 YYYZ=    31.1844 ZZZX=   -39.1267
 ZZZY=    28.8942 XXYY=  -953.4258 XXZZ=  -879.1135 YYZZ=  -624.9883
 XXYZ=    -7.2901 YYXZ=   -41.0542 ZZXY=    24.1907
 N-N= 1.864400880005D+03 E-N=-6.076979100859D+03  KE=
1.001667713180D+03
 1\1\GINC-OPT0075\FTS\RB3LYP\6-31+G(d)\C19H11N1O3\UCN0868\28-Sep-
2011\0
 \\# opt=(calcfc,ts) b3lyp/6-31+g(d) geom=connectivity\\cyanoDFT6-
31+d\
 \0,1\C,-0.5596560324,1.1340530675,-
0.7608935025\C,0.5341389752,0.44811
 83166,-1.4205627256\C,-
0.5639093145,1.0857965037,0.6590296323\C,0.4883

123206,0.3159544578,1.2864163353\H,0.4539010704,0.2330813455,2.3715301
 779\C,-0.0117647512,-1.6015888425,0.7437346711\H,0.7506222056,-
2.06549
 42306,1.3587553955\C,-0.0531567345,-1.712798483,-
0.6659788704\H,0.7132
 000551,-2.1342961394,-1.301246214\C,-1.6232331727,1.7670688814,-
1.4421
 082016\H,-1.6324266673,1.7848719519,-2.5279312052\C,-
2.6381179023,2.37
 11984857,-0.7192344219\H,-3.4444869965,2.8752451653,-1.244416322\C,-
2.
```

6408203657,2.3288472507,0.690650736\H,-
3.4487548538,2.800510778,1.2427
867392\C,-1.6278088874,1.6753033043,1.3730633794\H,-
1.6399088904,1.615

1809358,2.4579646427\C,1.7965859155,0.3406473807,0.6640621415\C,1.8243
173831,0.3820626817,-0.7534929679\C,3.0607547961,0.2872832833,-
1.42918
80845\H,3.0845450012,0.3105561344,-
2.5149347848\C,4.2380709136,0.18807
45176,-0.7042680514\H,5.1892044628,0.1409376418,-
1.2272158449\C,4.2111

090401,0.1478450657,0.7050495781\H,5.1412660652,0.0707153663,1.2612462

624\C,3.0019794749,0.204871532,1.3815856468\H,2.9751559089,0.163420691
,2.4679589305\C,-1.4698999668,-1.795264348,-1.0668953456\C,-
1.42900452
25,-1.6881461316,1.2116505683\O,-2.2545361167,-
1.6712782771,0.09952365
24\O,-1.8599424954,-1.7407538047,2.3336075902\O,-1.9788296527,-
1.94419
92924,-2.1444078837\C,0.5188768868,0.3521913065,-
2.8522006499\N,0.5313
574077,0.2726266938,-4.0131835335\\Version=AM64L-G03RevD.01\State=1-
A\
HF=-1011.0592935\RMSD=9.914e-09\RMSF=1.735e-
05\Thermal=0.\Dipole=1.962
547,1.0175608,1.526977\PG=C01 [X(C19H11N1O3)]\\@

CHILDREN YOU ARE VERY LITTLE,
AND YOUR BONES ARE VERY BRITTLE;
IF YOU WOULD GROW GREAT AND STATELY
YOU MUST TRY TO WALK SEDATELY.
YOU MUST STILL BE BRIGHT AND QUIET,
AND CONTENT WITH SIMPLE DIET;
AND REMAIN, THROUGH ALL BEWILD'RING
INNOCENT AND HONEST CHILDREN.
    -- A CHILD'S GARDEN OF VERSE,
       ROBERT LOUIS STEVENSON

Job cpu time: 1 days 5 hours 2 minutes 38.0 seconds.
File lengths (MBytes): RWF=   489 Int=   0 D2E=   0 Chk=
20 Scr=   1
Normal termination of Gaussian 03 at Wed Sep 28 20:16:15 2011.

This journal is © The Royal Society of Chemistry 2014

(15S)-9-cyano-9,10,11,15-tetrahydro-9,10-[3,4]furanoanthracene-12,14-dione

```
Entering Link 1 = C:\G09W\l1.exe PID=      6292.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2009, Gaussian, Inc.
                    All Rights Reserved.

 This is part of the Gaussian(R) 09 program.  It is based on
 the Gaussian(R) 03 system (copyright 2003, Gaussian, Inc.),
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

 This software contains proprietary and confidential information,
 including trade secrets, belonging to Gaussian, Inc.

 This software is provided under written license and may be
 used, copied, transmitted, or stored only in accord with that
 written license.

 The following legend is applicable only to US Government
 contracts under FAR:

                       RESTRICTED RIGHTS LEGEND

 Use, reproduction and disclosure by the US Government is
 subject to restrictions as set forth in subparagraphs (a)
 and (c) of the Commercial Computer Software - Restricted
 Rights clause in FAR 52.227-19.

 Gaussian, Inc.
 340 Quinnipiac St., Bldg. 40, Wallingford CT 06492


 ----------------------------------------------------------------
 Warning -- This program may not be used in any manner that
 competes with the business of Gaussian, Inc. or will provide
 assistance to any competitor of Gaussian, Inc.  The licensee
 of this program is prohibited from giving any competitor of
 Gaussian, Inc. access to this program.  By using this program,
 the user acknowledges that Gaussian, Inc. is engaged in the
```

```
 business of creating and licensing software in the field of
 computational chemistry and represents and warrants to the
 licensee that it is not a competitor of Gaussian, Inc. and that
 it will not use this program in any manner prohibited above.
 ----------------------------------------------------------------


 Cite this work as:
 Gaussian 09, Revision A.02,
 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
 M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
 G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
 A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
 M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
 Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
 J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
 K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand,
 K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
 M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
 V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
 O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
 R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
 P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
 O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
 and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

 ******************************************
 Gaussian 09:  IA32W-G09RevA.02 11-Jun-2009
               23-Jul-2013
 ******************************************
 %mem=64MW
 %chk=F:\solid state\Mack group papers\Ball mill energetics\James
Calculations\Cy
 anoAnthraceneCalculations\9-CYANODAPRODUCT2.chk
 ---------------------------------------
 # opt b3lyp/6-31+g(d) geom=connectivity
 ---------------------------------------
 1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
 2/9=110,12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
 4//1;
 5/5=2,38=5/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 7//1,2,3,16;
 1/14=-1,18=20,19=15/3(2);
 2/9=110/2;
 99//99;
 2/9=110/2;
 3/5=1,6=6,7=11,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
 4/5=5,16=3/1;
 5/5=2,38=5/2;
 7//1,2,3,16;
```

This journal is © The Royal Society of Chemistry 2014

```
 1/14=-1,18=20,19=15/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 ----------------
 9-cyanoDAproduct
 ----------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                    -1.66285  -1.06436  -0.02447
 C                    -0.23422  -1.57505  -0.04075
 H                    -0.16532  -2.66334   0.02221
 C                    -1.76284   0.3346   -0.09418
 C                     0.36549  -1.07056  -1.39996
 H                    -0.17062  -1.54858  -2.22485
 C                     0.52613  -0.87572   1.07206
 C                     0.44272   0.5259    1.0262
 C                    -0.39227   1.03176  -0.15778
 C                     0.30481   0.46703  -1.46635
 H                    -0.2407    0.83639  -2.33912
 C                     1.27454  -1.49471   2.06945
 H                     1.34899  -2.57851   2.10179
 C                     1.09896   1.3101    1.96946
 H                     1.03679   2.39334   1.92321
 C                     1.84007   0.68145   2.97584
 H                     2.35223   1.28493   3.71954
 C                     1.92832  -0.71018   3.02529
 H                     2.50961  -1.18926   3.80792
 C                    -2.81461  -1.84259   0.03182
 H                    -2.73914  -2.92589   0.08486
 C                    -4.06769  -1.21954   0.02622
 H                    -4.96958  -1.82298   0.07719
 C                    -4.16177   0.17045  -0.04235
 H                    -5.13651   0.64971  -0.04456
 C                    -3.00616   0.95767  -0.10605
 H                    -3.07881   2.04014  -0.15746
 C                     1.84488  -1.40008  -1.53291
 C                     1.76521   0.89643  -1.59348
 O                     2.58046  -0.22866  -1.64524
 O                     2.21534   2.00175  -1.65238
 O                     2.36606  -2.47721  -1.54153
 C                    -0.51681   2.48991  -0.2002
 N                    -0.66761   3.64026  -0.21208



GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Initialization pass.
                           ----------------------------
                           !    Initial Parameters    !
```

This journal is © The Royal Society of Chemistry 2014

! (Angstroms and Degrees) !

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.5173	estimate D2E/DX2
R2	R(1,4)	1.4043	estimate D2E/DX2
R3	R(1,20)	1.3912	estimate D2E/DX2
R4	R(2,3)	1.0923	estimate D2E/DX2
R5	R(2,5)	1.5689	estimate D2E/DX2
R6	R(2,7)	1.5184	estimate D2E/DX2
R7	R(4,9)	1.539	estimate D2E/DX2
R8	R(4,26)	1.3908	estimate D2E/DX2
R9	R(5,6)	1.0938	estimate D2E/DX2
R10	R(5,10)	1.5402	estimate D2E/DX2
R11	R(5,28)	1.5215	estimate D2E/DX2
R12	R(7,8)	1.4048	estimate D2E/DX2
R13	R(7,12)	1.3921	estimate D2E/DX2
R14	R(8,9)	1.5346	estimate D2E/DX2
R15	R(8,14)	1.3912	estimate D2E/DX2
R16	R(9,10)	1.5866	estimate D2E/DX2
R17	R(9,33)	1.4641	estimate D2E/DX2
R18	R(10,11)	1.0935	estimate D2E/DX2
R19	R(10,29)	1.5275	estimate D2E/DX2
R20	R(12,13)	1.0868	estimate D2E/DX2
R21	R(12,18)	1.3988	estimate D2E/DX2
R22	R(14,15)	1.086	estimate D2E/DX2

This journal is © The Royal Society of Chemistry 2014

```
 ! R23   R(14,16)              1.399          estimate D2E/DX2
!
 ! R24   R(16,17)              1.0861         estimate D2E/DX2
!
 ! R25   R(16,18)              1.3953         estimate D2E/DX2
!
 ! R26   R(18,19)              1.0862         estimate D2E/DX2
!
 ! R27   R(20,21)              1.0872         estimate D2E/DX2
!
 ! R28   R(20,22)              1.3994         estimate D2E/DX2
!
 ! R29   R(22,23)              1.0864         estimate D2E/DX2
!
 ! R30   R(22,24)              1.3949         estimate D2E/DX2
!
 ! R31   R(24,25)              1.0862         estimate D2E/DX2
!
 ! R32   R(24,26)              1.3997         estimate D2E/DX2
!
 ! R33   R(26,27)              1.0861         estimate D2E/DX2
!
 ! R34   R(28,30)              1.3878         estimate D2E/DX2
!
 ! R35   R(28,32)              1.1966         estimate D2E/DX2
!
 ! R36   R(29,30)              1.3904         estimate D2E/DX2
!
 ! R37   R(29,31)              1.1949         estimate D2E/DX2
!
 ! R38   R(33,34)              1.1603         estimate D2E/DX2
!
 ! A1    A(2,1,4)            113.6925         estimate D2E/DX2
!
 ! A2    A(2,1,20)           126.2772         estimate D2E/DX2
!
 ! A3    A(4,1,20)           120.0236         estimate D2E/DX2
!
 ! A4    A(1,2,3)            113.2116         estimate D2E/DX2
!
 ! A5    A(1,2,5)            105.1279         estimate D2E/DX2
!
 ! A6    A(1,2,7)            107.9759         estimate D2E/DX2
!
 ! A7    A(3,2,5)            110.2548         estimate D2E/DX2
!
 ! A8    A(3,2,7)            112.6475         estimate D2E/DX2
!
 ! A9    A(5,2,7)            107.1822         estimate D2E/DX2
!
 ! A10   A(1,4,9)            112.9499         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A11   A(1,4,26)             120.6901         estimate D2E/DX2
!
 ! A12   A(9,4,26)             126.3595         estimate D2E/DX2
!
 ! A13   A(2,5,6)              108.9943         estimate D2E/DX2
!
 ! A14   A(2,5,10)             110.077          estimate D2E/DX2
!
 ! A15   A(2,5,28)             112.1928         estimate D2E/DX2
!
 ! A16   A(6,5,10)             112.611          estimate D2E/DX2
!
 ! A17   A(6,5,28)             108.4228         estimate D2E/DX2
!
 ! A18   A(10,5,28)            104.5219         estimate D2E/DX2
!
 ! A19   A(2,7,8)              113.945          estimate D2E/DX2
!
 ! A20   A(2,7,12)             126.1208         estimate D2E/DX2
!
 ! A21   A(8,7,12)             119.9282         estimate D2E/DX2
!
 ! A22   A(7,8,9)              112.7292         estimate D2E/DX2
!
 ! A23   A(7,8,14)             120.8146         estimate D2E/DX2
!
 ! A24   A(9,8,14)             126.44           estimate D2E/DX2
!
 ! A25   A(4,9,8)              107.6596         estimate D2E/DX2
!
 ! A26   A(4,9,10)             105.3145         estimate D2E/DX2
!
 ! A27   A(4,9,33)             112.1237         estimate D2E/DX2
!
 ! A28   A(8,9,10)             106.257          estimate D2E/DX2
!
 ! A29   A(8,9,33)             113.3873         estimate D2E/DX2
!
 ! A30   A(10,9,33)            111.5914         estimate D2E/DX2
!
 ! A31   A(5,10,9)             109.7001         estimate D2E/DX2
!
 ! A32   A(5,10,11)            113.0331         estimate D2E/DX2
!
 ! A33   A(5,10,29)            104.2736         estimate D2E/DX2
!
 ! A34   A(9,10,11)            108.5954         estimate D2E/DX2
!
 ! A35   A(9,10,29)            112.8699         estimate D2E/DX2
!
 ! A36   A(11,10,29)           108.3947         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A37   A(7,12,13)            120.1014         estimate D2E/DX2
!
 ! A38   A(7,12,18)            119.4373         estimate D2E/DX2
!
 ! A39   A(13,12,18)           120.4612         estimate D2E/DX2
!
 ! A40   A(8,14,15)            120.423          estimate D2E/DX2
!
 ! A41   A(8,14,16)            118.9685         estimate D2E/DX2
!
 ! A42   A(15,14,16)           120.6084         estimate D2E/DX2
!
 ! A43   A(14,16,17)           119.5183         estimate D2E/DX2
!
 ! A44   A(14,16,18)           120.4754         estimate D2E/DX2
!
 ! A45   A(17,16,18)           120.0059         estimate D2E/DX2
!
 ! A46   A(12,18,16)           120.3722         estimate D2E/DX2
!
 ! A47   A(12,18,19)           119.6765         estimate D2E/DX2
!
 ! A48   A(16,18,19)           119.9511         estimate D2E/DX2
!
 ! A49   A(1,20,21)            120.1253         estimate D2E/DX2
!
 ! A50   A(1,20,22)            119.4786         estimate D2E/DX2
!
 ! A51   A(21,20,22)           120.3953         estimate D2E/DX2
!
 ! A52   A(20,22,23)           119.7279         estimate D2E/DX2
!
 ! A53   A(20,22,24)           120.2819         estimate D2E/DX2
!
 ! A54   A(23,22,24)           119.9902         estimate D2E/DX2
!
 ! A55   A(22,24,25)           120.0206         estimate D2E/DX2
!
 ! A56   A(22,24,26)           120.4647         estimate D2E/DX2
!
 ! A57   A(25,24,26)           119.5146         estimate D2E/DX2
!
 ! A58   A(4,26,24)            119.0597         estimate D2E/DX2
!
 ! A59   A(4,26,27)            120.4444         estimate D2E/DX2
!
 ! A60   A(24,26,27)           120.4947         estimate D2E/DX2
!
 ! A61   A(5,28,30)            109.855          estimate D2E/DX2
!
 ! A62   A(5,28,32)            128.2491         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A63   A(30,28,32)           121.8952         estimate D2E/DX2
!
 ! A64   A(10,29,30)           109.6463         estimate D2E/DX2
!
 ! A65   A(10,29,31)           128.6297         estimate D2E/DX2
!
 ! A66   A(30,29,31)           121.723          estimate D2E/DX2
!
 ! A67   A(28,30,29)           111.6689         estimate D2E/DX2
!
 ! A68   L(9,33,34,4,-1)       177.3681         estimate D2E/DX2
!
 ! A69   L(9,33,34,4,-2)       178.3808         estimate D2E/DX2
!
 ! D1    D(4,1,2,3)            179.518          estimate D2E/DX2
!
 ! D2    D(4,1,2,5)            -60.0748         estimate D2E/DX2
!
 ! D3    D(4,1,2,7)             54.0946         estimate D2E/DX2
!
 ! D4    D(20,1,2,3)            -1.4352         estimate D2E/DX2
!
 ! D5    D(20,1,2,5)           118.972          estimate D2E/DX2
!
 ! D6    D(20,1,2,7)          -126.8586         estimate D2E/DX2
!
 ! D7    D(2,1,4,9)             -0.5538         estimate D2E/DX2
!
 ! D8    D(2,1,4,26)           179.1985         estimate D2E/DX2
!
 ! D9    D(20,1,4,9)          -179.6663         estimate D2E/DX2
!
 ! D10   D(20,1,4,26)            0.0861         estimate D2E/DX2
!
 ! D11   D(2,1,20,21)            0.9491         estimate D2E/DX2
!
 ! D12   D(2,1,20,22)         -179.3643         estimate D2E/DX2
!
 ! D13   D(4,1,20,21)          179.941          estimate D2E/DX2
!
 ! D14   D(4,1,20,22)           -0.3725         estimate D2E/DX2
!
 ! D15   D(1,2,5,6)            -64.6189         estimate D2E/DX2
!
 ! D16   D(1,2,5,10)            59.349          estimate D2E/DX2
!
 ! D17   D(1,2,5,28)           175.2893         estimate D2E/DX2
!
 ! D18   D(3,2,5,6)             57.7215         estimate D2E/DX2
!
 ! D19   D(3,2,5,10)          -178.3106         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D20   D(3,2,5,28)           -62.3703         estimate D2E/DX2
!
 ! D21   D(7,2,5,6)           -179.3414         estimate D2E/DX2
!
 ! D22   D(7,2,5,10)           -55.3735         estimate D2E/DX2
!
 ! D23   D(7,2,5,28)            60.5668         estimate D2E/DX2
!
 ! D24   D(1,2,7,8)            -53.5386         estimate D2E/DX2
!
 ! D25   D(1,2,7,12)           127.3589         estimate D2E/DX2
!
 ! D26   D(3,2,7,8)           -179.2955         estimate D2E/DX2
!
 ! D27   D(3,2,7,12)             1.6021         estimate D2E/DX2
!
 ! D28   D(5,2,7,8)             59.261          estimate D2E/DX2
!
 ! D29   D(5,2,7,12)          -119.8414         estimate D2E/DX2
!
 ! D30   D(1,4,9,8)             -53.3533         estimate D2E/DX2
!
 ! D31   D(1,4,9,10)            59.7125         estimate D2E/DX2
!
 ! D32   D(1,4,9,33)          -178.7415         estimate D2E/DX2
!
 ! D33   D(26,4,9,8)           126.9111         estimate D2E/DX2
!
 ! D34   D(26,4,9,10)         -120.0231         estimate D2E/DX2
!
 ! D35   D(26,4,9,33)            1.5229         estimate D2E/DX2
!
 ! D36   D(1,4,26,24)            0.2377         estimate D2E/DX2
!
 ! D37   D(1,4,26,27)          179.8407         estimate D2E/DX2
!
 ! D38   D(9,4,26,24)          179.9546         estimate D2E/DX2
!
 ! D39   D(9,4,26,27)           -0.4424         estimate D2E/DX2
!
 ! D40   D(2,5,10,9)            -1.9901         estimate D2E/DX2
!
 ! D41   D(2,5,10,11)         -123.3409         estimate D2E/DX2
!
 ! D42   D(2,5,10,29)          119.144          estimate D2E/DX2
!
 ! D43   D(6,5,10,9)           119.8538         estimate D2E/DX2
!
 ! D44   D(6,5,10,11)           -1.497          estimate D2E/DX2
!
 ! D45   D(6,5,10,29)         -119.0121         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D46   D(28,5,10,9)         -122.661          estimate D2E/DX2
!
 ! D47   D(28,5,10,11)         115.9881         estimate D2E/DX2
!
 ! D48   D(28,5,10,29)          -1.527          estimate D2E/DX2
!
 ! D49   D(2,5,28,30)         -118.5224         estimate D2E/DX2
!
 ! D50   D(2,5,28,32)           61.177          estimate D2E/DX2
!
 ! D51   D(6,5,28,30)          121.054          estimate D2E/DX2
!
 ! D52   D(6,5,28,32)          -59.2466         estimate D2E/DX2
!
 ! D53   D(10,5,28,30)           0.7295         estimate D2E/DX2
!
 ! D54   D(10,5,28,32)        -179.571          estimate D2E/DX2
!
 ! D55   D(2,7,8,9)             -0.6438         estimate D2E/DX2
!
 ! D56   D(2,7,8,14)          -179.2678         estimate D2E/DX2
!
 ! D57   D(12,7,8,9)           178.5196         estimate D2E/DX2
!
 ! D58   D(12,7,8,14)           -0.1044         estimate D2E/DX2
!
 ! D59   D(2,7,12,13)           -0.3445         estimate D2E/DX2
!
 ! D60   D(2,7,12,18)          179.5967         estimate D2E/DX2
!
 ! D61   D(8,7,12,13)         -179.398          estimate D2E/DX2
!
 ! D62   D(8,7,12,18)            0.5433         estimate D2E/DX2
!
 ! D63   D(7,8,9,4)             53.9153         estimate D2E/DX2
!
 ! D64   D(7,8,9,10)           -58.515          estimate D2E/DX2
!
 ! D65   D(7,8,9,33)           178.5468         estimate D2E/DX2
!
 ! D66   D(14,8,9,4)          -127.5537         estimate D2E/DX2
!
 ! D67   D(14,8,9,10)          120.016          estimate D2E/DX2
!
 ! D68   D(14,8,9,33)           -2.9222         estimate D2E/DX2
!
 ! D69   D(7,8,14,15)          179.4981         estimate D2E/DX2
!
 ! D70   D(7,8,14,16)           -0.4332         estimate D2E/DX2
!
 ! D71   D(9,8,14,15)            1.0757         estimate D2E/DX2
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D72   D(9,8,14,16)         -178.8555         estimate D2E/DX2
!
 ! D73   D(4,9,10,5)           -55.9862         estimate D2E/DX2
!
 ! D74   D(4,9,10,11)           67.9966         estimate D2E/DX2
!
 ! D75   D(4,9,10,29)         -171.7873         estimate D2E/DX2
!
 ! D76   D(8,9,10,5)            58.0607         estimate D2E/DX2
!
 ! D77   D(8,9,10,11)         -177.9565         estimate D2E/DX2
!
 ! D78   D(8,9,10,29)          -57.7405         estimate D2E/DX2
!
 ! D79   D(33,9,10,5)         -177.8777         estimate D2E/DX2
!
 ! D80   D(33,9,10,11)         -53.8949         estimate D2E/DX2
!
 ! D81   D(33,9,10,29)          66.3212         estimate D2E/DX2
!
 ! D82   D(5,10,29,30)           1.9044         estimate D2E/DX2
!
 ! D83   D(5,10,29,31)        -178.4638         estimate D2E/DX2
!
 ! D84   D(9,10,29,30)         120.905          estimate D2E/DX2
!
 ! D85   D(9,10,29,31)          -59.4632         estimate D2E/DX2
!
 ! D86   D(11,10,29,30)       -118.764          estimate D2E/DX2
!
 ! D87   D(11,10,29,31)         60.8678         estimate D2E/DX2
!
 ! D88   D(7,12,18,16)          -0.4451         estimate D2E/DX2
!
 ! D89   D(7,12,18,19)         179.7215         estimate D2E/DX2
!
 ! D90   D(13,12,18,16)        179.4959         estimate D2E/DX2
!
 ! D91   D(13,12,18,19)         -0.3375         estimate D2E/DX2
!
 ! D92   D(8,14,16,17)        -179.7218         estimate D2E/DX2
!
 ! D93   D(8,14,16,18)           0.5326         estimate D2E/DX2
!
 ! D94   D(15,14,16,17)          0.347          estimate D2E/DX2
!
 ! D95   D(15,14,16,18)       -179.3985         estimate D2E/DX2
!
 ! D96   D(14,16,18,12)         -0.0965         estimate D2E/DX2
!
 ! D97   D(14,16,18,19)        179.7364         estimate D2E/DX2
!
```

```
 ! D98   D(17,16,18,12)       -179.8408         estimate D2E/DX2
!
 ! D99   D(17,16,18,19)         -0.008          estimate D2E/DX2
!
 ! D100  D(1,20,22,23)        -179.5654         estimate D2E/DX2
!
 ! D101  D(1,20,22,24)           0.3361         estimate D2E/DX2
!
 ! D102  D(21,20,22,23)          0.1203         estimate D2E/DX2
!
 ! D103  D(21,20,22,24)       -179.9783         estimate D2E/DX2
!
 ! D104  D(20,22,24,25)       -179.8861         estimate D2E/DX2
!
 ! D105  D(20,22,24,26)         -0.0112         estimate D2E/DX2
!
 ! D106  D(23,22,24,25)          0.0151         estimate D2E/DX2
!
 ! D107  D(23,22,24,26)        179.89           estimate D2E/DX2
!
 ! D108  D(22,24,26,4)          -0.2747         estimate D2E/DX2
!
 ! D109  D(22,24,26,27)       -179.8775         estimate D2E/DX2
!
 ! D110  D(25,24,26,4)         179.6009         estimate D2E/DX2
!
 ! D111  D(25,24,26,27)         -0.0019         estimate D2E/DX2
!
 ! D112  D(5,28,30,29)           0.492          estimate D2E/DX2
!
 ! D113  D(32,28,30,29)       -179.23           estimate D2E/DX2
!
 ! D114  D(10,29,30,28)         -1.543          estimate D2E/DX2
!
 ! D115  D(31,29,30,28)        178.7952         estimate D2E/DX2
!
 ---------------------------------------------------------------------
-----------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
 Number of steps in this run= 204 maximum allowed number of steps=
204.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.662851   -1.064359   -0.024468
      2          6           0       -0.234215   -1.575049   -0.040752
```

This journal is © The Royal Society of Chemistry 2014

3	1	0	-0.165321	-2.663335	0.022207
4	6	0	-1.762837	0.334602	-0.094182
5	6	0	0.365485	-1.070561	-1.399958
6	1	0	-0.170616	-1.548583	-2.224847
7	6	0	0.526130	-0.875717	1.072057
8	6	0	0.442724	0.525901	1.026197
9	6	0	-0.392270	1.031761	-0.157780
10	6	0	0.304806	0.467026	-1.466350
11	1	0	-0.240701	0.836389	-2.339124
12	6	0	1.274538	-1.494706	2.069448
13	1	0	1.348985	-2.578509	2.101787
14	6	0	1.098957	1.310099	1.969463
15	1	0	1.036793	2.393338	1.923210
16	6	0	1.840072	0.681449	2.975835
17	1	0	2.352232	1.284929	3.719542
18	6	0	1.928316	-0.710182	3.025288
19	1	0	2.509611	-1.189262	3.807921
20	6	0	-2.814608	-1.842590	0.031817
21	1	0	-2.739136	-2.925891	0.084859
22	6	0	-4.067686	-1.219536	0.026220
23	1	0	-4.969582	-1.822982	0.077188
24	6	0	-4.161767	0.170450	-0.042353
25	1	0	-5.136514	0.649705	-0.044560
26	6	0	-3.006163	0.957674	-0.106053
27	1	0	-3.078811	2.040140	-0.157464
28	6	0	1.844879	-1.400079	-1.532911
29	6	0	1.765208	0.896427	-1.593483
30	8	0	2.580455	-0.228659	-1.645241
31	8	0	2.215335	2.001753	-1.652384
32	8	0	2.366064	-2.477206	-1.541525
33	6	0	-0.516805	2.489908	-0.200197
34	7	0	-0.667605	3.640264	-0.212077

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.517257	0.000000			
3	H	2.191232	1.092280	0.000000		
4	C	1.404261	2.446693	3.399004	0.000000	
5	C	2.450746	1.568945	2.200281	2.865186	0.000000
6	H	2.702389	2.185181	2.508376	3.259032	1.093778
7	C	2.455522	1.518398	2.185376	2.839781	2.484880
8	C	2.840118	2.451656	3.398373	2.481198	2.905320
9	C	2.454764	2.614218	3.706432	1.539003	2.556747
10	C	2.880250	2.548126	3.497997	2.485061	1.540215
11	H	3.315567	3.331304	4.222515	2.758342	2.210419
12	C	3.632896	2.595329	2.762261	4.153710	3.611517
13	H	3.985570	2.846740	2.573902	4.794990	3.937435
14	C	4.152276	3.760637	4.601998	3.660613	4.190289
15	H	4.799708	4.606593	5.534332	4.018233	4.846926
16	C	4.931545	4.300494	4.892147	4.746184	4.938776
17	H	5.971403	5.386000	5.966335	5.690466	5.975347

18	C	4.724715	3.850342	4.149291	4.944419	4.706922
19	H	5.666767	4.742330	4.864132	5.983509	5.633238
20	C	1.391171	2.595240	2.773524	2.421211	3.571974
21	H	2.153054	2.848716	2.587931	3.408230	3.909681
22	C	2.410369	3.850503	4.160892	2.782476	4.659311
23	H	3.394159	4.743320	4.877514	3.868818	5.586684
24	C	2.787410	4.297957	4.899601	2.405098	4.886636
25	H	3.873597	5.383501	5.974400	3.388724	5.921859
26	C	2.428942	3.755349	4.604187	1.390762	4.141973
27	H	3.414754	4.601624	5.535647	2.155145	4.804522
28	C	3.833051	2.565109	2.838153	4.253783	1.521468
29	C	4.249480	3.537917	4.359966	3.874358	2.421924
30	O	4.618544	3.508492	4.030796	4.646206	2.382237
31	O	5.204948	4.625058	5.498620	4.586201	3.595105
32	O	4.530977	3.134910	2.981243	5.200855	2.449695
33	C	3.738598	4.077886	5.170002	2.491822	3.859378
34	N	4.812400	5.236093	6.327917	3.484370	4.966911

		6	7	8	9	10
6	H	0.000000				
7	C	3.436245	0.000000			
8	C	3.904991	1.404846	0.000000		
9	C	3.313619	2.448352	1.534572	0.000000	
10	C	2.205453	2.880183	2.497054	1.586567	0.000000
11	H	2.388737	3.893006	3.448022	2.195314	1.093500
12	C	4.531263	1.392139	2.421392	3.757902	4.158202
13	H	4.699968	2.153354	3.408161	4.601267	4.805954
14	C	5.232219	2.431308	1.391172	2.612737	3.625777
15	H	5.848329	3.416425	2.155196	2.868211	3.966812
16	C	6.005248	2.788473	2.403719	3.863368	4.704894
17	H	7.051901	3.874560	3.387691	4.757101	5.635104
18	C	5.715973	2.410112	2.780512	4.307134	4.918985
19	H	6.611128	3.393738	3.866755	5.392647	5.951671
20	C	3.488505	3.630079	4.148343	3.763717	4.160478
21	H	3.718738	3.979917	4.788029	4.607566	4.814947
22	C	4.512508	4.723889	4.938654	4.314033	4.918429
23	H	5.329609	5.664797	5.975862	5.399681	5.953639
24	C	4.862884	4.930796	4.740199	3.868370	4.697446
25	H	5.852031	5.969865	5.682407	4.760949	5.626973
26	C	4.337158	4.150465	3.655576	2.615454	3.612985
27	H	5.060692	4.796826	4.011880	2.869552	3.954331
28	C	2.136129	2.966465	3.496351	3.579059	2.421226
29	C	3.181840	3.432333	2.957867	2.595047	1.527522
30	O	3.105887	3.467368	3.503689	3.555038	2.386327
31	O	4.315711	4.307647	3.534839	3.158216	2.457665
32	O	2.786398	3.575043	4.394438	4.672901	3.594849
33	C	4.530835	3.746168	2.506404	1.464070	2.523933
34	N	5.587698	4.844387	3.530639	2.623556	3.547989

		11	12	13	14	15
11	H	0.000000				
12	C	5.212050	0.000000			
13	H	5.823257	1.086838	0.000000		
14	C	4.536850	2.812073	3.898884	0.000000	

This journal is © The Royal Society of Chemistry 2014

15	H	4.714188	3.898050	4.984839	1.086007	0.000000
16	C	5.709852	2.424256	3.410638	1.399013	2.164218
17	H	6.605446	3.407434	4.306947	2.152698	2.487119
18	C	5.989443	1.398761	2.163128	2.425724	3.411924
19	H	7.032328	2.154296	2.487560	3.408325	4.307708
20	C	4.407186	4.581930	4.707638	5.386085	6.029407
21	H	5.125683	4.700688	4.571806	6.018829	6.777269
22	C	4.946463	5.726243	5.957777	6.072022	6.535070
23	H	5.939119	6.562461	6.677882	7.086894	7.567146
24	C	4.592754	6.065135	6.520928	5.746427	5.985791
25	H	5.410070	7.083016	7.555784	6.585857	6.709851
26	C	3.556557	5.391788	6.028803	4.613456	4.746002
27	H	3.776708	6.033732	6.785390	4.744526	4.625165
28	C	3.162501	3.648456	3.853004	4.490889	5.194977
29	C	2.140854	4.401743	5.089542	3.648232	3.890817
30	O	3.094305	4.136086	4.591136	4.198654	4.689521
31	O	2.803890	5.192529	5.985245	3.852591	3.785125
32	O	4.290839	3.898187	3.783971	5.317544	6.123198
33	C	2.717603	4.923144	5.871044	2.951281	2.632841
34	N	3.545179	5.945182	6.934965	3.648222	3.003206

		16	17	18	19	20
16	C	0.000000				
17	H	1.086092	0.000000			
18	C	1.395303	2.154568	0.000000		
19	H	2.154114	2.480766	1.086249	0.000000	
20	C	6.058388	7.076505	5.721761	6.559962	0.000000
21	H	6.506903	7.540819	5.944796	6.665314	1.087221
22	C	6.871359	7.818460	6.723533	7.587029	1.399440
23	H	7.813176	8.748418	7.583575	8.382022	2.155541
24	C	6.737407	7.604347	6.875685	7.821810	2.423359
25	H	7.602404	8.405551	7.822089	8.757091	3.407142
26	C	5.749811	6.592016	6.077510	7.095935	2.810192
27	H	5.988240	6.715486	6.539534	7.575208	3.896309
28	C	4.966042	5.920721	4.610867	5.386167	4.935079
29	C	4.574985	5.359456	4.892938	5.837756	5.578398
30	O	4.767684	5.578883	4.740358	5.537576	5.875713
31	O	4.827467	5.421270	5.414572	6.331201	6.551018
32	O	5.537175	6.467819	4.916277	5.504178	5.451376
33	C	4.348859	5.004768	5.159743	6.225793	4.909610
34	N	5.020539	5.488592	6.012131	7.041265	5.893284

		21	22	23	24	25
21	H	0.000000				
22	C	2.163361	0.000000			
23	H	2.488244	1.086352	0.000000		
24	C	3.409896	1.394853	2.154211	0.000000	
25	H	4.306862	2.154406	2.481304	1.086196	0.000000
26	C	3.897413	2.425813	3.408906	1.399714	2.153374
27	H	4.983529	3.411320	4.307411	2.163743	2.486000
28	C	5.094946	6.117345	7.014852	6.384992	7.426752
29	C	6.141340	6.412752	7.452766	6.169447	7.077697
30	O	6.210182	6.926283	7.906433	6.941621	7.930026
31	O	7.200449	7.257463	8.321241	6.827393	7.646098

This journal is © The Royal Society of Chemistry 2014

32	O	5.376756	6.740378	7.540553	7.202095	8.264814
33	C	5.860963	5.140038	6.205255	4.323257	4.975166
34	N	6.891575	5.935907	6.959722	4.927229	5.379838

		26	27	28	29	30
26	C	0.000000				
27	H	1.086119	0.000000			
28	C	5.579205	6.161955	0.000000		
29	C	4.998218	5.180227	2.298686	0.000000	
30	O	5.914963	6.276004	1.387773	1.390369	0.000000
31	O	5.544843	5.501295	3.424029	1.194918	2.260111
32	O	6.536039	7.208932	1.196625	3.427116	2.261125
33	C	2.924638	2.601536	4.741906	3.112557	4.367125
34	N	3.560391	2.894356	5.784655	3.918610	5.250944

		31	32	33	34
31	O	0.000000			
32	O	4.482865	0.000000		
33	C	3.132368	5.897653	0.000000	
34	N	3.615321	6.956581	1.160259	0.000000

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.662851	-1.064359	-0.024468
2	6	0	-0.234215	-1.575049	-0.040752
3	1	0	-0.165321	-2.663335	0.022207
4	6	0	-1.762837	0.334602	-0.094182
5	6	0	0.365485	-1.070561	-1.399958
6	1	0	-0.170616	-1.548583	-2.224847
7	6	0	0.526130	-0.875717	1.072057
8	6	0	0.442724	0.525901	1.026197
9	6	0	-0.392270	1.031761	-0.157780
10	6	0	0.304806	0.467026	-1.466350
11	1	0	-0.240701	0.836389	-2.339124
12	6	0	1.274538	-1.494706	2.069448
13	1	0	1.348985	-2.578509	2.101787
14	6	0	1.098957	1.310099	1.969463
15	1	0	1.036793	2.393338	1.923210
16	6	0	1.840072	0.681449	2.975835
17	1	0	2.352232	1.284929	3.719542
18	6	0	1.928316	-0.710182	3.025288
19	1	0	2.509611	-1.189262	3.807921
20	6	0	-2.814608	-1.842590	0.031817
21	1	0	-2.739136	-2.925891	0.084859
22	6	0	-4.067686	-1.219536	0.026220
23	1	0	-4.969582	-1.822982	0.077188

```
     24          6           0       -4.161767    0.170450   -0.042353
     25          1           0       -5.136514    0.649705   -0.044560
     26          6           0       -3.006163    0.957674   -0.106053
     27          1           0       -3.078811    2.040140   -0.157464
     28          6           0        1.844879   -1.400079   -1.532911
     29          6           0        1.765208    0.896427   -1.593483
     30          8           0        2.580455   -0.228659   -1.645241
     31          8           0        2.215335    2.001753   -1.652384
     32          8           0        2.366064   -2.477206   -1.541525
     33          6           0       -0.516805    2.489908   -0.200197
     34          7           0       -0.667605    3.640264   -0.212077
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3785120      0.2690514
0.2564356
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1881.8498939798 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A)
 The electronic state of the initial guess is 1-A.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1011.11144876     A.U. after   16 cycles
            Convg  =    0.5461D-08             -V/T =  2.0093


**********************************************************************

            Population analysis using the SCF density.

**********************************************************************

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A)
       Virtual  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.24754 -19.18782 -19.18736 -14.36203 -
10.36097
 Alpha  occ. eigenvalues --  -10.36047 -10.29065 -10.26521 -10.25800 -
10.25161
 Alpha  occ. eigenvalues --  -10.24939 -10.23728 -10.23460 -10.23248 -
10.22982
 Alpha  occ. eigenvalues --  -10.22399 -10.22295 -10.22162 -10.22046 -
10.22036
 Alpha  occ. eigenvalues --  -10.21989 -10.21796 -10.21700  -1.16504
-1.10009
 Alpha  occ. eigenvalues --   -1.06154  -0.95015  -0.92389  -0.88433
-0.86679
 Alpha  occ. eigenvalues --   -0.83718  -0.80901  -0.77822  -0.77256
-0.76165
 Alpha  occ. eigenvalues --   -0.71566  -0.69788  -0.66329  -0.65567
-0.63272
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha  occ. eigenvalues --   -0.63189  -0.60058  -0.58538  -0.56397
-0.54898
 Alpha  occ. eigenvalues --   -0.53487  -0.51221  -0.50872  -0.49863
-0.49291
 Alpha  occ. eigenvalues --   -0.48447  -0.47760  -0.46693  -0.46489
-0.46331
 Alpha  occ. eigenvalues --   -0.45994  -0.45232  -0.44846  -0.44087
-0.42251
 Alpha  occ. eigenvalues --   -0.41105  -0.40794  -0.39028  -0.38820
-0.38616
 Alpha  occ. eigenvalues --   -0.38018  -0.37581  -0.36858  -0.36252
-0.35479
 Alpha  occ. eigenvalues --   -0.35050  -0.34698  -0.32954  -0.30293
-0.28536
 Alpha  occ. eigenvalues --   -0.28179  -0.27841  -0.26630
 Alpha virt. eigenvalues --   -0.05836  -0.04995  -0.04632  -0.04385
-0.02652
 Alpha virt. eigenvalues --   -0.02490  -0.01250  -0.00252  -0.00036
 0.00581
 Alpha virt. eigenvalues --    0.00746   0.01149   0.02409   0.02577
 0.03060
 Alpha virt. eigenvalues --    0.03188   0.03656   0.04590   0.04794
 0.05110
 Alpha virt. eigenvalues --    0.05974   0.06053   0.06389   0.07440
 0.07700
 Alpha virt. eigenvalues --    0.08063   0.08718   0.09155   0.09214
 0.09453
 Alpha virt. eigenvalues --    0.09997   0.10211   0.10839   0.11033
 0.11203
 Alpha virt. eigenvalues --    0.11731   0.12221   0.12521   0.12841
 0.13170
 Alpha virt. eigenvalues --    0.13457   0.13890   0.14055   0.14338
 0.14763
 Alpha virt. eigenvalues --    0.15074   0.15275   0.15582   0.15931
 0.16271
 Alpha virt. eigenvalues --    0.16555   0.16891   0.17224   0.17808
 0.17999
 Alpha virt. eigenvalues --    0.18552   0.18698   0.18852   0.19220
 0.19567
 Alpha virt. eigenvalues --    0.19730   0.20234   0.20420   0.20541
 0.20766
 Alpha virt. eigenvalues --    0.21236   0.21383   0.21674   0.22032
 0.22434
 Alpha virt. eigenvalues --    0.22611   0.23143   0.23382   0.23689
 0.24013
 Alpha virt. eigenvalues --    0.24408   0.24567   0.24691   0.24979
 0.25687
 Alpha virt. eigenvalues --    0.25875   0.26243   0.26542   0.26902
 0.27029
 Alpha virt. eigenvalues --    0.27375   0.27557   0.27585   0.28101
 0.28498
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.28990   0.29325   0.29501   0.29792
0.30195
 Alpha virt. eigenvalues --    0.30582   0.30931   0.31075   0.31637
0.32310
 Alpha virt. eigenvalues --    0.32665   0.32909   0.33398   0.33743
0.34052
 Alpha virt. eigenvalues --    0.34622   0.35027   0.35445   0.35845
0.36507
 Alpha virt. eigenvalues --    0.36729   0.37428   0.37940   0.38309
0.39286
 Alpha virt. eigenvalues --    0.39969   0.40073   0.40688   0.41134
0.41588
 Alpha virt. eigenvalues --    0.42053   0.43349   0.43606   0.44298
0.44643
 Alpha virt. eigenvalues --    0.45536   0.46894   0.50069   0.52080
0.55597
 Alpha virt. eigenvalues --    0.56378   0.57588   0.59412   0.61290
0.62691
 Alpha virt. eigenvalues --    0.66410   0.67232   0.68124   0.68576
0.69533
 Alpha virt. eigenvalues --    0.70186   0.70608   0.71084   0.71751
0.72107
 Alpha virt. eigenvalues --    0.72156   0.73019   0.73910   0.74668
0.75209
 Alpha virt. eigenvalues --    0.75654   0.76228   0.76576   0.76930
0.78058
 Alpha virt. eigenvalues --    0.79354   0.79776   0.79873   0.80384
0.80771
 Alpha virt. eigenvalues --    0.81409   0.82709   0.83258   0.84028
0.84855
 Alpha virt. eigenvalues --    0.85717   0.86321   0.87215   0.88413
0.88879
 Alpha virt. eigenvalues --    0.89268   0.89909   0.90885   0.91573
0.92491
 Alpha virt. eigenvalues --    0.93808   0.93867   0.95497   0.95754
0.95997
 Alpha virt. eigenvalues --    0.97453   0.98641   0.99328   1.00122
1.01122
 Alpha virt. eigenvalues --    1.02180   1.03156   1.04174   1.04352
1.05156
 Alpha virt. eigenvalues --    1.06867   1.07921   1.08102   1.09185
1.09396
 Alpha virt. eigenvalues --    1.11869   1.12507   1.14084   1.14769
1.16000
 Alpha virt. eigenvalues --    1.17177   1.17910   1.18373   1.20757
1.21124
 Alpha virt. eigenvalues --    1.21604   1.22485   1.23622   1.24721
1.26084
 Alpha virt. eigenvalues --    1.27300   1.28438   1.30033   1.31410
1.32399
 Alpha virt. eigenvalues --    1.34103   1.34558   1.35155   1.35226
1.36722
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    1.37851   1.38337   1.39329   1.40369
1.41596
 Alpha virt. eigenvalues --    1.41893   1.42680   1.43240   1.43797
1.45104
 Alpha virt. eigenvalues --    1.45606   1.46261   1.47688   1.47965
1.48549
 Alpha virt. eigenvalues --    1.49490   1.51107   1.52809   1.53891
1.55630
 Alpha virt. eigenvalues --    1.57893   1.58968   1.60322   1.62855
1.63487
 Alpha virt. eigenvalues --    1.67236   1.69126   1.69352   1.69831
1.72066
 Alpha virt. eigenvalues --    1.75108   1.76342   1.77159   1.77692
1.79496
 Alpha virt. eigenvalues --    1.80021   1.81085   1.82158   1.82654
1.83430
 Alpha virt. eigenvalues --    1.84639   1.85453   1.85955   1.86685
1.87996
 Alpha virt. eigenvalues --    1.88382   1.89676   1.90435   1.91807
1.93118
 Alpha virt. eigenvalues --    1.93417   1.95078   1.96229   1.97002
1.97393
 Alpha virt. eigenvalues --    1.98025   1.98766   2.00002   2.00872
2.02283
 Alpha virt. eigenvalues --    2.02350   2.03340   2.04645   2.05619
2.07483
 Alpha virt. eigenvalues --    2.08777   2.11112   2.12076   2.12593
2.15331
 Alpha virt. eigenvalues --    2.17116   2.17588   2.18613   2.20049
2.20762
 Alpha virt. eigenvalues --    2.23590   2.24373   2.25432   2.26075
2.27672
 Alpha virt. eigenvalues --    2.28388   2.29546   2.30755   2.31605
2.34717
 Alpha virt. eigenvalues --    2.35626   2.37121   2.39106   2.41315
2.43182
 Alpha virt. eigenvalues --    2.46060   2.49250   2.49878   2.52007
2.54102
 Alpha virt. eigenvalues --    2.56783   2.58853   2.59625   2.62221
2.63271
 Alpha virt. eigenvalues --    2.64814   2.67694   2.68335   2.69087
2.69312
 Alpha virt. eigenvalues --    2.71700   2.73211   2.75014   2.75224
2.77323
 Alpha virt. eigenvalues --    2.79029   2.80091   2.80338   2.82925
2.83932
 Alpha virt. eigenvalues --    2.84344   2.85751   2.90243   2.94086
2.94985
 Alpha virt. eigenvalues --    2.96123   3.03978   3.05717   3.09801
3.12759
 Alpha virt. eigenvalues --    3.15496   3.22759   3.23136   3.27150
3.33260
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    3.34775   3.40511   3.45604   4.23213
4.25721
 Alpha virt. eigenvalues --    4.27048   4.30572   4.32875   4.34435
4.35767
 Alpha virt. eigenvalues --    4.38606   4.42279   4.43718   4.47822
4.48296
 Alpha virt. eigenvalues --    4.49437   4.51785   4.56976   4.62212
4.67080
 Alpha virt. eigenvalues --    4.73729   4.75878   4.81672   4.89320
5.15711
 Alpha virt. eigenvalues --    5.47557
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   15.098628  -3.852447  -0.035049   1.475523  -0.040724
0.026772
     2  C   -3.852447  22.197175   0.225800  -7.043173  -2.198531  -
0.033375
     3  H   -0.035049   0.225800   0.524492   0.004295   0.002645  -
0.002888
     4  C    1.475523  -7.043173   0.004295  27.248448   1.619828
0.020920
     5  C   -0.040724  -2.198531   0.002645   1.619828  11.318903
0.322801
     6  H    0.026772  -0.033375  -0.002888   0.020920   0.322801
0.474370
     7  C   -0.074353  -3.894056  -0.067935   0.348888   0.544636
0.020193
     8  C    3.957417 -10.253381   0.017049   0.557579   1.463165
0.009181
     9  C   -2.283201   5.919885  -0.011132  -2.878813  -2.241409  -
0.008892
    10  C    1.143939   0.104676   0.030110  -1.458760  -2.947980  -
0.009643
    11  H   -0.045387  -0.004589  -0.000113   0.085731  -0.025561  -
0.004233
    12  C   -0.437617   2.157829   0.040787  -0.946952   0.078586
0.009298
    13  H   -0.016579  -0.040373   0.003253  -0.001563  -0.009650  -
0.000006
    14  C   -2.085522   2.515862   0.001677   0.968199  -0.055072
0.001247
    15  H   -0.002759   0.006350   0.000002   0.000875   0.001797
0.000000
    16  C   -0.070988  -0.161722   0.001604  -0.018401  -0.023624
0.000016
    17  H    0.002285   0.002528   0.000000  -0.003673   0.000960
0.000000
    18  C   -0.317301   0.304574   0.008034  -0.040385  -0.048131
0.001333
    19  H   -0.002628  -0.015988  -0.000004   0.001723  -0.000527
0.000000
```

This journal is © The Royal Society of Chemistry 2014

20	C	-0.852022	0.035798	0.030778	-3.662346	0.458515	-0.030356
21	H	-0.020648	-0.080383	0.003329	0.087071	0.011560	-0.000055
22	C	-1.189240	-0.912972	0.004047	-0.703068	0.039989	-0.004972
23	H	0.014368	-0.013360	-0.000004	0.023371	-0.001469	0.000001
24	C	0.023173	0.622311	-0.001800	1.847661	-0.111230	0.004645
25	H	0.008744	0.002934	0.000000	0.023886	0.000726	0.000000
26	C	1.069138	-0.509755	0.011851	-10.842324	-0.176544	-0.004199
27	H	0.031170	-0.005413	0.000002	-0.105227	-0.001078	0.000000
28	C	-0.657061	0.794699	-0.018900	-0.498028	-1.221284	-0.072957
29	C	-0.397328	0.733952	-0.000736	-0.351631	0.493454	0.009919
30	O	0.007903	0.121953	-0.000415	-0.011819	-0.351033	0.005185
31	O	0.023791	-0.066338	0.000073	0.020520	-0.028407	-0.000637
32	O	0.027048	-0.119194	0.004901	0.017376	-0.006563	-0.002248
33	C	-4.065054	-1.192052	0.008518	0.095805	-0.510634	0.012222
34	N	0.087767	0.061446	-0.000026	-0.103267	0.023562	-0.000146

		7	8	9	10	11	12
1	C	-0.074353	3.957417	-2.283201	1.143939	-0.045387	-0.437617
2	C	-3.894056	-10.253381	5.919885	0.104676	-0.004589	2.157829
3	H	-0.067935	0.017049	-0.011132	0.030110	-0.000113	0.040787
4	C	0.348888	0.557579	-2.878813	-1.458760	0.085731	-0.946952
5	C	0.544636	1.463165	-2.241409	-2.947980	-0.025561	0.078586
6	H	0.020193	0.009181	-0.008892	-0.009643	-0.004233	0.009298
7	C	16.373660	3.457421	-2.857742	0.199397	0.004099	-3.997541
8	C	3.457421	43.528784	-5.162341	-2.020370	-0.000079	-5.998786
9	C	-2.857742	-5.162341	19.765993	0.565263	0.012811	0.422673
10	C	0.199397	-2.020370	0.565263	11.977803	0.326980	-0.089678

This journal is © The Royal Society of Chemistry 2014

```
    11  H    0.004099  -0.000079   0.012811   0.326980   0.460000  -
0.002709
    12  C   -3.997541  -5.998786   0.422673  -0.089678  -0.002709
10.130435
    13  H   -0.074261   0.059320   0.024301  -0.000911   0.000000
0.288136
    14  C   -1.484421 -20.110003   1.139665   0.211246   0.023732
3.914476
    15  H    0.038308  -0.153665  -0.033511  -0.017877  -0.000005  -
0.006793
    16  C    0.768086   0.338477  -0.257448   0.147906   0.000656  -
1.293929
    17  H    0.014027   0.038337  -0.013504  -0.000358   0.000000
0.015333
    18  C   -1.583930  -1.714689   0.238486  -0.014329   0.000216
1.245237
    19  H    0.021985   0.035356   0.003333   0.000822   0.000000  -
0.010013
    20  C    1.267313   0.307719  -1.778082  -0.140234  -0.013893  -
0.405454
    21  H    0.007363   0.008822   0.003706  -0.002271   0.000000
0.000014
    22  C    0.124799   0.463241  -0.460074   0.012846  -0.004686  -
0.201911
    23  H   -0.003018   0.000469   0.004465   0.001179   0.000000
0.000511
    24  C   -0.102146  -1.164703   0.130259   0.370533   0.007533
0.162188
    25  H    0.000703  -0.004495  -0.012524  -0.000357   0.000001  -
0.000197
    26  C    0.536603   3.242962  -0.625412   0.009901  -0.049382  -
0.420465
    27  H    0.001918   0.021809  -0.041943  -0.001450  -0.000059
0.001001
    28  C   -0.749655  -0.976328   1.050680   0.373827   0.024573
0.353348
    29  C   -0.201438  -0.751484  -0.031484  -0.942304  -0.076113
0.218231
    30  O   -0.102300  -0.156052   0.076730  -0.186099   0.004850
0.016859
    31  O   -0.012123   0.189783  -0.029018  -0.148096  -0.000744  -
0.010066
    32  O    0.126314   0.073331  -0.054094  -0.061608  -0.000661  -
0.082443
    33  C   -2.432418  -3.225679  -4.939294  -1.424096   0.004921
0.526375
    34  N    0.113177  -0.177400   0.133265  -0.023240   0.001390
0.012465
             13         14         15         16         17         18
     1  C   -0.016579  -2.085522  -0.002759  -0.070988   0.002285  -
0.317301
```

This journal is © The Royal Society of Chemistry 2014

```
     2  C   -0.040373   2.515862   0.006350  -0.161722   0.002528
0.304574
     3  H    0.003253   0.001677   0.000002   0.001604   0.000000
0.008034
     4  C   -0.001563   0.968199   0.000875  -0.018401  -0.003673  -
0.040385
     5  C   -0.009650  -0.055072   0.001797  -0.023624   0.000960  -
0.048131
     6  H   -0.000006   0.001247   0.000000   0.000016   0.000000
0.001333
     7  C   -0.074261  -1.484421   0.038308   0.768086   0.014027  -
1.583930
     8  C    0.059320 -20.110003  -0.153665   0.338477   0.038337  -
1.714689
     9  C    0.024301   1.139665  -0.033511  -0.257448  -0.013504
0.238486
    10  C   -0.000911   0.211246  -0.017877   0.147906  -0.000358  -
0.014329
    11  H    0.000000   0.023732  -0.000005   0.000656   0.000000
0.000216
    12  C    0.288136   3.914476  -0.006793  -1.293929   0.015333
1.245237
    13  H    0.530277  -0.014380   0.000018   0.005430  -0.000158
0.049220
    14  C   -0.014380  21.602999   0.353919  -1.828183  -0.018765
0.604823
    15  H    0.000018   0.353919   0.503056   0.063119  -0.003904
0.014413
    16  C    0.005430  -1.828183   0.063119   8.085888   0.323727
0.698126
    17  H   -0.000158  -0.018765  -0.003904   0.323727   0.518501  -
0.058349
    18  C    0.049220   0.604823   0.014413   0.698126  -0.058349
6.628330
    19  H   -0.004222  -0.001192  -0.000150  -0.042928  -0.004216
0.306772
    20  C   -0.006669  -0.640463   0.000743  -0.023149  -0.000072  -
0.090658
    21  H    0.000000   0.000351   0.000000  -0.000183   0.000000
0.000528
    22  C   -0.000796  -0.279439  -0.000096  -0.010694   0.000029  -
0.039956
    23  H    0.000000  -0.000116   0.000000  -0.000017   0.000000
0.000007
    24  C   -0.000038   0.536081  -0.001032  -0.014808  -0.000021
0.037469
    25  H    0.000000   0.000726   0.000000   0.000006   0.000000
0.000009
    26  C    0.000220  -2.340678  -0.006871  -0.011884   0.000754  -
0.101934
    27  H    0.000000  -0.006650   0.000001  -0.000719   0.000000  -
0.000030
```

This journal is © The Royal Society of Chemistry 2014

28	C	0.015648	0.657027	-0.000471	-0.022729	-0.001234
0.043291						
29	C	-0.000996	0.192835	0.014985	-0.033557	0.001604
0.044997						
30	O	-0.000124	0.034770	-0.000122	-0.017024	-0.000008
0.009667						
31	O	0.000000	-0.125314	-0.000402	-0.016450	-0.000047
-0.005691						
32	O	-0.000335	-0.034563	-0.000002	0.001449	0.000003
-0.015925						
33	C	0.004079	2.453336	0.011007	-0.161303	-0.005602
0.047127						
34	N	-0.000001	0.054898	0.005757	0.019238	0.000088
0.003889						

		19	20	21	22	23	24
1	C	-0.002628	-0.852022	-0.020648	-1.189240	0.014368	
0.023173							
2	C	-0.015988	0.035798	-0.080383	-0.912972	-0.013360	
0.622311							
3	H	-0.000004	0.030778	0.003329	0.004047	-0.000004	
-0.001800							
4	C	0.001723	-3.662346	0.087071	-0.703068	0.023371	
1.847661							
5	C	-0.000527	0.458515	0.011560	0.039989	-0.001469	
-0.111230							
6	H	0.000000	-0.030356	-0.000055	-0.004972	0.000001	
0.004645							
7	C	0.021985	1.267313	0.007363	0.124799	-0.003018	
-0.102146							
8	C	0.035356	0.307719	0.008822	0.463241	0.000469	
-1.164703							
9	C	0.003333	-1.778082	0.003706	-0.460074	0.004465	
0.130259							
10	C	0.000822	-0.140234	-0.002271	0.012846	0.001179	
0.370533							
11	H	0.000000	-0.013893	0.000000	-0.004686	0.000000	
0.007533							
12	C	-0.010013	-0.405454	0.000014	-0.201911	0.000511	
0.162188							
13	H	-0.004222	-0.006669	0.000000	-0.000796	0.000000	
-0.000038							
14	C	-0.001192	-0.640463	0.000351	-0.279439	-0.000116	
0.536081							
15	H	-0.000150	0.000743	0.000000	-0.000096	0.000000	
-0.001032							
16	C	-0.042928	-0.023149	-0.000183	-0.010694	-0.000017	
-0.014808							
17	H	-0.004216	-0.000072	0.000000	0.000029	0.000000	
-0.000021							
18	C	0.306772	-0.090658	0.000528	-0.039956	0.000007	
0.037469							

This journal is © The Royal Society of Chemistry 2014

19	H	0.521863	0.000429	0.000000	0.000008	0.000000	-0.000006
20	C	0.000429	9.838890	0.260363	1.045073	-0.016216	-1.405489
21	H	0.000000	0.260363	0.533518	0.018738	-0.004221	0.005220
22	C	0.000008	1.045073	0.018738	7.121964	0.310303	0.321281
23	H	0.000000	-0.016216	-0.004221	0.310303	0.522609	-0.028658
24	C	-0.000006	-1.405489	0.005220	0.321281	-0.028658	8.809559
25	H	0.000000	0.021251	-0.000157	-0.039931	-0.004209	0.326568
26	C	-0.000210	2.710477	-0.022826	0.883217	0.004705	-4.661249
27	H	0.000000	-0.007212	0.000018	0.021895	-0.000149	0.051139
28	C	0.001103	-0.286327	0.001536	-0.041689	0.000002	0.038483
29	C	-0.001016	-0.002542	-0.000480	-0.029821	-0.000062	0.074839
30	O	-0.000008	0.019765	0.000000	0.003386	0.000000	-0.002630
31	O	0.000004	0.002225	0.000000	0.000501	0.000000	-0.002934
32	O	-0.000032	0.022175	0.000003	0.000462	0.000000	-0.000597
33	C	0.000142	-0.860471	0.002814	-0.156443	0.000410	0.524861
34	N	-0.000002	0.011396	-0.000006	-0.006548	0.000001	0.014382

		25	26	27	28	29	30
1	C	0.008744	1.069138	0.031170	-0.657061	-0.397328	0.007903
2	C	0.002934	-0.509755	-0.005413	0.794699	0.733952	0.121953
3	H	0.000000	0.011851	0.000002	-0.018900	-0.000736	-0.000415
4	C	0.023886	-10.842324	-0.105227	-0.498028	-0.351631	-0.011819
5	C	0.000726	-0.176544	-0.001078	-1.221284	0.493454	-0.351033
6	H	0.000000	-0.004199	0.000000	-0.072957	0.009919	0.005185
7	C	0.000703	0.536603	0.001918	-0.749655	-0.201438	-0.102300
8	C	-0.004495	3.242962	0.021809	-0.976328	-0.751484	-0.156052
9	C	-0.012524	-0.625412	-0.041943	1.050680	-0.031484	0.076730

This journal is © The Royal Society of Chemistry 2014

10	C	-0.000357	0.009901	-0.001450	0.373827	-0.942304	-0.186099
11	H	0.000001	-0.049382	-0.000059	0.024573	-0.076113	0.004850
12	C	-0.000197	-0.420465	0.001001	0.353348	0.218231	0.016859
13	H	0.000000	0.000220	0.000000	0.015648	-0.000996	-0.000124
14	C	0.000726	-2.340678	-0.006650	0.657027	0.192835	0.034770
15	H	0.000000	-0.006871	0.000001	-0.000471	0.014985	-0.000122
16	C	0.000006	-0.011884	-0.000719	-0.022729	-0.033557	-0.017024
17	H	0.000000	0.000754	0.000000	-0.001234	0.001604	-0.000008
18	C	0.000009	-0.101934	-0.000030	0.043291	0.044997	0.009667
19	H	0.000000	-0.000210	0.000000	0.001103	-0.001016	-0.000008
20	C	0.021251	2.710477	-0.007212	-0.286327	-0.002542	0.019765
21	H	-0.000157	-0.022826	0.000018	0.001536	-0.000480	0.000000
22	C	-0.039931	0.883217	0.021895	-0.041689	-0.029821	0.003386
23	H	-0.004209	0.004705	-0.000149	0.000002	-0.000062	0.000000
24	C	0.326568	-4.661249	0.051139	0.038483	0.074839	-0.002630
25	H	0.519415	-0.025471	-0.003934	-0.000075	0.000002	0.000000
26	C	-0.025471	19.813313	0.334050	-0.197872	-0.014054	0.011864
27	H	-0.003934	0.334050	0.501277	-0.000520	0.002222	0.000000
28	C	-0.000075	-0.197872	-0.000520	6.737937	-0.733243	0.223338
29	C	0.000002	-0.014054	0.002222	-0.733243	6.367366	0.282718
30	O	0.000000	0.011864	0.000000	0.223338	0.282718	8.357211
31	O	0.000000	0.000572	0.000004	0.026992	0.517573	-0.068140
32	O	0.000000	0.004521	0.000000	0.431121	0.032145	-0.080535
33	C	-0.004641	-2.234864	-0.009285	0.349936	0.324659	0.031676
34	N	0.000136	-0.024016	0.004278	-0.000688	-0.000535	-0.000839

		31	32	33	34
1	C	0.023791	0.027048	-4.065054	0.087767

This journal is © The Royal Society of Chemistry 2014

2	C	-0.066338	-0.119194	-1.192052	0.061446
3	H	0.000073	0.004901	0.008518	-0.000026
4	C	0.020520	0.017376	0.095805	-0.103267
5	C	-0.028407	-0.006563	-0.510634	0.023562
6	H	-0.000637	-0.002248	0.012222	-0.000146
7	C	-0.012123	0.126314	-2.432418	0.113177
8	C	0.189783	0.073331	-3.225679	-0.177400
9	C	-0.029018	-0.054094	-4.939294	0.133265
10	C	-0.148096	-0.061608	-1.424096	-0.023240
11	H	-0.000744	-0.000661	0.004921	0.001390
12	C	-0.010066	-0.082443	0.526375	0.012465
13	H	0.000000	-0.000335	0.004079	-0.000001
14	C	-0.125314	-0.034563	2.453336	0.054898
15	H	-0.000402	-0.000002	0.011007	0.005757
16	C	-0.016450	0.001449	-0.161303	0.019238
17	H	-0.000047	0.000003	-0.005602	0.000088
18	C	-0.005691	-0.015925	0.047127	0.003889
19	H	0.000004	-0.000032	0.000142	-0.000002
20	C	0.002225	0.022175	-0.860471	0.011396
21	H	0.000000	0.000003	0.002814	-0.000006
22	C	0.000501	0.000462	-0.156443	-0.006548
23	H	0.000000	0.000000	0.000410	0.000001
24	C	-0.002934	-0.000597	0.524861	0.014382
25	H	0.000000	0.000000	-0.004641	0.000136
26	C	0.000572	0.004521	-2.234864	-0.024016
27	H	0.000004	0.000000	-0.009285	0.004278
28	C	0.026992	0.431121	0.349936	-0.000688
29	C	0.517573	0.032145	0.324659	-0.000535
30	O	-0.068140	-0.080535	0.031676	-0.000839
31	O	8.049740	0.000179	0.024553	-0.003814
32	O	0.000179	8.100435	-0.012014	0.000086
33	C	0.024553	-0.012014	22.557315	0.284632
34	N	-0.003814	0.000086	0.284632	6.838848

Mulliken atomic charges:

		1
1	C	-0.551759
2	C	0.589328
3	H	0.215754
4	C	0.221731
5	C	-0.381680
6	H	0.256505
7	C	-0.331552
8	C	0.099234
9	C	0.228405
10	C	0.013231
11	H	0.270722
12	C	0.310771
13	H	0.191160
14	C	-0.243108
15	H	0.213309
16	C	-0.443989
17	H	0.191733

This journal is © The Royal Society of Chemistry 2014

```
    18  C   -0.255239
    19  H    0.189602
    20  C    0.188746
    21  H    0.186279
    22  C   -0.289444
    23  H    0.189095
    24  C   -0.410841
    25  H    0.190884
    26  C   -0.364140
    27  H    0.212886
    28  C    0.355520
    29  C    0.257321
    30  O   -0.230728
    31  O   -0.338289
    32  O   -0.370736
    33  C   -0.030537
    34  N   -0.330176
 Sum of Mulliken atomic charges =   0.00000
 Mulliken charges with hydrogens summed into heavy atoms:
               1
     1  C   -0.551759
     2  C    0.805082
     4  C    0.221731
     5  C   -0.125174
     7  C   -0.331552
     8  C    0.099234
     9  C    0.228405
    10  C    0.283953
    12  C    0.501931
    14  C   -0.029799
    16  C   -0.252256
    18  C   -0.065637
    20  C    0.375024
    22  C   -0.100348
    24  C   -0.219957
    26  C   -0.151255
    28  C    0.355520
    29  C    0.257321
    30  O   -0.230728
    31  O   -0.338289
    32  O   -0.370736
    33  C   -0.030537
    34  N   -0.330176
 Sum of Mulliken charges with hydrogens summed into heavy atoms =
0.00000
 Electronic spatial extent (au):  <R**2>=           5237.0780
 Charge=              0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=             -4.2486    Y=             -3.9599    Z=
1.4792  Tot=              5.9933
 Quadrupole moment (field-independent basis, Debye-Ang):
```

```
   XX=           -134.0466   YY=           -148.3078   ZZ=           -
125.0842
   XY=              5.0952   XZ=             12.4975   YZ=
0.9580
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=              1.7663   YY=            -12.4949   ZZ=
10.7287
   XY=              5.0952   XZ=             12.4975   YZ=
0.9580
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=            -68.5961  YYY=            -82.1312  ZZZ=
-15.1927  XYY=           -18.1602
  XXY=              0.9704  XXZ=             29.2621  XZZ=
31.9108  YZZ=              0.3215
  YYZ=             27.9705  XYZ=             -1.6528
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=          -3234.1163 YYYY=          -2305.5032 ZZZZ=          -
1676.4911 XXXY=             29.2903
 XXXZ=             41.0747 YYYX=             98.2222 YYYZ=
4.5844 ZZZX=            56.1788
 ZZZY=             12.0379 XXYY=           -925.7233 XXZZ=           -
886.9708 YYZZ=           -629.8847
 XXYZ=            -13.8848 YYXZ=             58.2975 ZZXY=
-6.8085
 N-N= 1.881849893980D+03 E-N=-6.111844525884D+03  KE=
1.001826934995D+03
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.001194695    0.000195014   -0.000259492
      2        6           0.000045508   -0.000169881    0.000328139
      3        1          -0.000236060   -0.000169279    0.000206207
      4        6           0.000951575    0.000002263   -0.000241227
      5        6           0.000394361   -0.000207819    0.000056737
      6        1          -0.000009663   -0.000189812   -0.000251922
      7        6          -0.000624475    0.000012198   -0.000680146
      8        6          -0.000417937   -0.000032287   -0.000450564
      9        6          -0.000034101    0.000056006    0.000215067
     10        6           0.000296559    0.000504135   -0.000210967
     11        1          -0.000039912    0.000115733   -0.000276240
     12        6          -0.000272368   -0.001030242   -0.000029379
     13        1           0.000101404   -0.000348696    0.000026103
     14        6          -0.000505137    0.000787341   -0.000157185
     15        1           0.000192501    0.000353393    0.000104649
     16        6           0.000533816    0.000865042    0.000876961
     17        1           0.000150590    0.000154338    0.000168403
     18        6           0.000593332   -0.000633061    0.000933944
     19        1           0.000175075   -0.000100190    0.000180288
```

20	6	0.000443923	-0.001169521	0.000094972
21	1	-0.000054847	-0.000353157	0.000027998
22	6	-0.001188678	-0.000656585	0.000037667
23	1	-0.000223690	-0.000126105	0.000020771
24	6	-0.001307052	0.000579984	0.000013888
25	1	-0.000231220	0.000108620	0.000005891
26	6	0.000379043	0.001029238	-0.000040041
27	1	-0.000287898	0.000274718	-0.000001809
28	6	-0.002000854	0.002076980	0.000058879
29	6	-0.001329913	-0.000871141	0.000323325
30	8	0.000924203	-0.000514445	-0.000186568
31	8	0.001225599	0.001300867	-0.000699638
32	8	0.001603449	-0.002246688	-0.000440305
33	6	-0.000283053	-0.000157888	0.000337082
34	7	-0.000158774	0.000560927	-0.000091486

Cartesian Forces: Max 0.002246688 RMS 0.000641670

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Internal Forces: Max 0.002720629 RMS 0.000452502
Search for a local minimum.
Step number 1 out of a maximum of 204
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Second derivative matrix not updated -- first step.
Eigenvalues --- 0.00429 0.00678 0.00776 0.01149
0.01171
Eigenvalues --- 0.01206 0.01426 0.01482 0.01580
0.01818
Eigenvalues --- 0.02114 0.02118 0.02128 0.02129
0.02130
Eigenvalues --- 0.02130 0.02151 0.02151 0.02159
0.02162
Eigenvalues --- 0.02166 0.02169 0.02840 0.03423
0.04188
Eigenvalues --- 0.04836 0.04863 0.04863 0.05259
0.05338
Eigenvalues --- 0.05503 0.06453 0.06656 0.07487
0.08538
Eigenvalues --- 0.08803 0.09716 0.10035 0.12247
0.16000
Eigenvalues --- 0.16000 0.16000 0.16000 0.16000
0.16000
Eigenvalues --- 0.16000 0.16000 0.16297 0.20390
0.21840
Eigenvalues --- 0.22000 0.22000 0.22294 0.22613
0.22632
Eigenvalues --- 0.24523 0.24584 0.24604 0.24999
0.25000

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.26099   0.27401   0.27634   0.28757
0.28896
     Eigenvalues ---    0.29706   0.29911   0.34380   0.34411
0.34550
     Eigenvalues ---    0.35136   0.35181   0.35238   0.35250
0.35256
     Eigenvalues ---    0.35265   0.35268   0.35278   0.36459
0.37044
     Eigenvalues ---    0.40156   0.42089   0.42129   0.43472
0.44176
     Eigenvalues ---    0.44596   0.45996   0.46026   0.46123
0.46482
     Eigenvalues ---    0.46521   0.46889   0.46989   1.06538
1.07419
     Eigenvalues ---
1.276241000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 RFO step:  Lambda=-2.11092571D-04 EMin= 4.28709935D-03
 Linear search not attempted -- first point.
 Iteration  1 RMS(Cart)=  0.01349110 RMS(Int)=  0.00013149
 Iteration  2 RMS(Cart)=  0.00013186 RMS(Int)=  0.00005029
 Iteration  3 RMS(Cart)=  0.00000003 RMS(Int)=  0.00005029
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (Linear)    (Quad)   (Total)
    R1        2.86720  -0.00007   0.00000  -0.00068  -0.00069
2.86651
    R2        2.65367   0.00062   0.00000   0.00168   0.00167
2.65533
    R3        2.62893   0.00146   0.00000   0.00303   0.00303
2.63196
    R4        2.06411   0.00017   0.00000   0.00048   0.00048
2.06459
    R5        2.96488   0.00078   0.00000   0.00279   0.00279
2.96767
    R6        2.86936   0.00027   0.00000   0.00100   0.00100
2.87036
    R7        2.90829   0.00029   0.00000   0.00199   0.00199
2.91028
    R8        2.62816   0.00151   0.00000   0.00317   0.00317
2.63133
    R9        2.06694   0.00028   0.00000   0.00081   0.00081
2.06775
   R10        2.91059   0.00104   0.00000   0.00273   0.00273
2.91331
   R11        2.87516   0.00004   0.00000  -0.00034  -0.00038
2.87478
   R12        2.65477   0.00090   0.00000   0.00171   0.00172
2.65649
   R13        2.63076   0.00133   0.00000   0.00283   0.00283
2.63359
   R14        2.89992   0.00062   0.00000   0.00167   0.00167
2.90159
   R15        2.62893   0.00133   0.00000   0.00278   0.00278
2.63172
```

This journal is © The Royal Society of Chemistry 2014

R16	2.99818	0.00122	0.00000	0.00499	0.00500
3.00318					
R17	2.76669	0.00043	0.00000	0.00119	0.00119
2.76788					
R18	2.06641	0.00028	0.00000	0.00082	0.00082
2.06723					
R19	2.88660	0.00056	0.00000	0.00202	0.00206
2.88866					
R20	2.05383	0.00036	0.00000	0.00101	0.00101
2.05484					
R21	2.64328	0.00144	0.00000	0.00317	0.00317
2.64645					
R22	2.05226	0.00034	0.00000	0.00095	0.00095
2.05321					
R23	2.64375	0.00139	0.00000	0.00304	0.00304
2.64679					
R24	2.05242	0.00027	0.00000	0.00077	0.00077
2.05318					
R25	2.63674	0.00145	0.00000	0.00315	0.00315
2.63989					
R26	2.05271	0.00027	0.00000	0.00076	0.00076
2.05347					
R27	2.05455	0.00035	0.00000	0.00100	0.00100
2.05555					
R28	2.64456	0.00159	0.00000	0.00350	0.00350
2.64806					
R29	2.05291	0.00026	0.00000	0.00073	0.00073
2.05364					
R30	2.63589	0.00135	0.00000	0.00300	0.00300
2.63889					
R31	2.05261	0.00026	0.00000	0.00072	0.00072
2.05334					
R32	2.64508	0.00158	0.00000	0.00353	0.00353
2.64860					
R33	2.05247	0.00029	0.00000	0.00083	0.00083
2.05330					
R34	2.62251	-0.00002	0.00000	0.00019	0.00016
2.62267					
R35	2.26129	0.00272	0.00000	0.00255	0.00255
2.26385					
R36	2.62742	0.00059	0.00000	0.00171	0.00173
2.62915					
R37	2.25807	0.00170	0.00000	0.00158	0.00158
2.25965					
R38	2.19257	0.00058	0.00000	0.00045	0.00045
2.19302					
A1	1.98431	0.00020	0.00000	0.00000	0.00000
1.98431					
A2	2.20395	-0.00034	0.00000	-0.00069	-0.00069
2.20326					
A3	2.09481	0.00014	0.00000	0.00072	0.00072
2.09553					

This journal is © The Royal Society of Chemistry 2014

A4	1.97591	-0.00012	0.00000	-0.00235	-0.00236
1.97355					
A5	1.83483	-0.00019	0.00000	-0.00357	-0.00356
1.83127					
A6	1.88454	-0.00013	0.00000	-0.00157	-0.00156
1.88298					
A7	1.92431	0.00003	0.00000	0.00250	0.00249
1.92680					
A8	1.96607	-0.00003	0.00000	-0.00006	-0.00007
1.96600					
A9	1.87068	0.00047	0.00000	0.00520	0.00518
1.87586					
A10	1.97135	-0.00006	0.00000	0.00052	0.00053
1.97187					
A11	2.10644	-0.00006	0.00000	-0.00078	-0.00078
2.10566					
A12	2.20539	0.00012	0.00000	0.00027	0.00026
2.20565					
A13	1.90231	-0.00013	0.00000	-0.00122	-0.00120
1.90111					
A14	1.92121	-0.00004	0.00000	0.00074	0.00073
1.92194					
A15	1.95813	0.00044	0.00000	0.00494	0.00493
1.96306					
A16	1.96543	0.00010	0.00000	-0.00149	-0.00151
1.96393					
A17	1.89234	-0.00034	0.00000	-0.00375	-0.00376
1.88858					
A18	1.82425	-0.00002	0.00000	0.00091	0.00092
1.82517					
A19	1.98872	0.00003	0.00000	0.00070	0.00069
1.98940					
A20	2.20122	-0.00012	0.00000	-0.00074	-0.00075
2.20048					
A21	2.09314	0.00010	0.00000	0.00013	0.00013
2.09327					
A22	1.96750	-0.00008	0.00000	-0.00037	-0.00037
1.96712					
A23	2.10861	-0.00004	0.00000	-0.00015	-0.00015
2.10847					
A24	2.20679	0.00012	0.00000	0.00061	0.00061
2.20740					
A25	1.87901	-0.00016	0.00000	-0.00183	-0.00182
1.87719					
A26	1.83808	-0.00018	0.00000	-0.00146	-0.00145
1.83664					
A27	1.95693	-0.00019	0.00000	-0.00335	-0.00336
1.95357					
A28	1.85453	0.00035	0.00000	0.00292	0.00290
1.85744					
A29	1.97898	0.00000	0.00000	0.00072	0.00071
1.97969					

This journal is © The Royal Society of Chemistry 2014

A30	1.94764	0.00019	0.00000	0.00302	0.00302
1.95065					
A31	1.91463	-0.00018	0.00000	-0.00150	-0.00151
1.91312					
A32	1.97280	0.00008	0.00000	-0.00192	-0.00195
1.97085					
A33	1.81992	-0.00026	0.00000	-0.00149	-0.00143
1.81849					
A34	1.89535	-0.00012	0.00000	-0.00121	-0.00119
1.89415					
A35	1.96995	0.00074	0.00000	0.00888	0.00884
1.97880					
A36	1.89184	-0.00024	0.00000	-0.00253	-0.00256
1.88929					
A37	2.09617	0.00004	0.00000	0.00021	0.00021
2.09637					
A38	2.08457	0.00004	0.00000	0.00030	0.00030
2.08488					
A39	2.10244	-0.00008	0.00000	-0.00051	-0.00051
2.10193					
A40	2.10178	0.00017	0.00000	0.00116	0.00116
2.10294					
A41	2.07639	0.00012	0.00000	0.00052	0.00052
2.07691					
A42	2.10501	-0.00029	0.00000	-0.00168	-0.00168
2.10333					
A43	2.08599	0.00005	0.00000	0.00020	0.00020
2.08619					
A44	2.10269	-0.00011	0.00000	-0.00041	-0.00041
2.10228					
A45	2.09450	0.00005	0.00000	0.00021	0.00021
2.09470					
A46	2.10089	-0.00012	0.00000	-0.00037	-0.00037
2.10052					
A47	2.08875	0.00007	0.00000	0.00029	0.00029
2.08903					
A48	2.09354	0.00004	0.00000	0.00008	0.00008
2.09362					
A49	2.09658	0.00005	0.00000	0.00043	0.00043
2.09702					
A50	2.08529	0.00007	0.00000	0.00014	0.00014
2.08544					
A51	2.10130	-0.00011	0.00000	-0.00058	-0.00058
2.10072					
A52	2.08965	0.00009	0.00000	0.00037	0.00037
2.09001					
A53	2.09931	-0.00015	0.00000	-0.00050	-0.00051
2.09881					
A54	2.09422	0.00006	0.00000	0.00014	0.00014
2.09436					
A55	2.09476	0.00006	0.00000	0.00011	0.00011
2.09487					

This journal is © The Royal Society of Chemistry 2014

A56	2.10251	-0.00014	0.00000	-0.00032	-0.00032	2.10219
A57	2.08592	0.00008	0.00000	0.00020	0.00020	2.08612
A58	2.07798	0.00015	0.00000	0.00074	0.00074	2.07873
A59	2.10215	0.00020	0.00000	0.00136	0.00136	2.10351
A60	2.10303	-0.00035	0.00000	-0.00211	-0.00211	2.10092
A61	1.91733	0.00027	0.00000	0.00001	-0.00009	1.91725
A62	2.23837	0.00044	0.00000	0.00234	0.00220	2.24057
A63	2.12747	-0.00071	0.00000	-0.00222	-0.00236	2.12511
A64	1.91369	0.00004	0.00000	0.00002	-0.00018	1.91351
A65	2.24501	0.00075	0.00000	0.00293	0.00248	2.24749
A66	2.12447	-0.00079	0.00000	-0.00323	-0.00367	2.12080
A67	1.94899	-0.00004	0.00000	0.00014	0.00028	1.94927
A68	3.09566	-0.00018	0.00000	-0.00367	-0.00367	3.09199
A69	3.11333	0.00012	0.00000	0.00235	0.00235	3.11569
D1	3.13318	-0.00010	0.00000	-0.00056	-0.00056	3.13262
D2	-1.04850	-0.00025	0.00000	-0.00117	-0.00116	-1.04966
D3	0.94413	0.00014	0.00000	0.00236	0.00236	0.94649
D4	-0.02505	-0.00002	0.00000	0.00152	0.00152	-0.02353
D5	2.07645	-0.00018	0.00000	0.00092	0.00093	2.07738
D6	-2.21410	0.00021	0.00000	0.00445	0.00445	-2.20965
D7	-0.00967	-0.00002	0.00000	-0.00229	-0.00229	-0.01195
D8	3.12760	0.00008	0.00000	0.00240	0.00239	3.13000
D9	-3.13577	-0.00008	0.00000	-0.00421	-0.00421	-3.13998
D10	0.00150	0.00001	0.00000	0.00047	0.00047	0.00197
D11	0.01657	-0.00005	0.00000	-0.00132	-0.00132	0.01525
D12	-3.13050	-0.00008	0.00000	-0.00213	-0.00212	-3.13262

This journal is © The Royal Society of Chemistry 2014

D13	3.14056	0.00003	0.00000	0.00088	0.00088	3.14144
D14	-0.00650	0.00001	0.00000	0.00007	0.00007	-0.00643
D15	-1.12781	0.00015	0.00000	0.00919	0.00919	-1.11862
D16	1.03584	0.00016	0.00000	0.00699	0.00699	1.04282
D17	3.05938	0.00038	0.00000	0.01157	0.01159	3.07096
D18	1.00743	-0.00010	0.00000	0.00557	0.00557	1.01300
D19	-3.11211	-0.00009	0.00000	0.00337	0.00337	-3.10874
D20	-1.08857	0.00013	0.00000	0.00796	0.00797	-1.08060
D21	-3.13010	0.00018	0.00000	0.01034	0.01035	-3.11974
D22	-0.96645	0.00019	0.00000	0.00814	0.00815	-0.95830
D23	1.05709	0.00041	0.00000	0.01272	0.01275	1.06984
D24	-0.93443	-0.00004	0.00000	-0.00051	-0.00050	-0.93493
D25	2.22283	-0.00013	0.00000	-0.00684	-0.00684	2.21600
D26	-3.12930	0.00024	0.00000	0.00375	0.00375	-3.12555
D27	0.02796	0.00015	0.00000	-0.00258	-0.00258	0.02538
D28	1.03430	-0.00009	0.00000	-0.00285	-0.00285	1.03145
D29	-2.09163	-0.00019	0.00000	-0.00918	-0.00919	-2.10081
D30	-0.93119	-0.00006	0.00000	0.00056	0.00056	-0.93063
D31	1.04218	0.00018	0.00000	0.00241	0.00240	1.04457
D32	-3.11963	0.00018	0.00000	0.00324	0.00323	-3.11639
D33	2.21502	-0.00016	0.00000	-0.00444	-0.00444	2.21058
D34	-2.09480	0.00008	0.00000	-0.00259	-0.00260	-2.09740
D35	0.02658	0.00009	0.00000	-0.00176	-0.00176	0.02482
D36	0.00415	-0.00001	0.00000	-0.00062	-0.00062	0.00353
D37	3.13881	-0.00004	0.00000	-0.00206	-0.00206	3.13675
D38	3.14080	0.00009	0.00000	0.00473	0.00473	-3.13765

This journal is © The Royal Society of Chemistry 2014

D39	-0.00772	0.00006	0.00000	0.00330	0.00329	-0.00443
D40	-0.03473	-0.00009	0.00000	-0.00729	-0.00730	-0.04203
D41	-2.15271	0.00013	0.00000	-0.00337	-0.00338	-2.15608
D42	2.07945	0.00054	0.00000	0.00156	0.00154	2.08100
D43	2.09184	-0.00022	0.00000	-0.00935	-0.00935	2.08250
D44	-0.02613	0.00001	0.00000	-0.00543	-0.00543	-0.03156
D45	-2.07715	0.00041	0.00000	-0.00050	-0.00051	-2.07766
D46	-2.14084	-0.00058	0.00000	-0.01405	-0.01405	-2.15489
D47	2.02437	-0.00036	0.00000	-0.01013	-0.01014	2.01424
D48	-0.02665	0.00004	0.00000	-0.00521	-0.00522	-0.03187
D49	-2.06861	-0.00023	0.00000	-0.00662	-0.00661	-2.07521
D50	1.06774	0.00006	0.00000	0.02313	0.02314	1.09088
D51	2.11279	-0.00012	0.00000	-0.00568	-0.00567	2.10712
D52	-1.03405	0.00017	0.00000	0.02406	0.02408	-1.00997
D53	0.01273	-0.00006	0.00000	-0.00258	-0.00255	0.01018
D54	-3.13411	0.00023	0.00000	0.02717	0.02720	-3.10691
D55	-0.01124	-0.00001	0.00000	-0.00157	-0.00157	-0.01281
D56	-3.12881	-0.00009	0.00000	-0.00569	-0.00570	-3.13451
D57	3.11575	0.00008	0.00000	0.00433	0.00433	3.12008
D58	-0.00182	0.00000	0.00000	0.00020	0.00020	-0.00162
D59	-0.00601	0.00011	0.00000	0.00628	0.00628	0.00027
D60	3.13455	0.00008	0.00000	0.00500	0.00500	3.13955
D61	-3.13109	0.00001	0.00000	-0.00040	-0.00040	-3.13148
D62	0.00948	-0.00002	0.00000	-0.00168	-0.00168	0.00780
D63	0.94100	0.00004	0.00000	0.00113	0.00113	0.94213
D64	-1.02128	0.00016	0.00000	0.00225	0.00225	-1.01903

This journal is © The Royal Society of Chemistry 2014

D65	3.11623	-0.00033	0.00000	-0.00405	-0.00406	3.11217
D66	-2.22623	0.00012	0.00000	0.00552	0.00552	-2.22071
D67	2.09467	0.00024	0.00000	0.00665	0.00664	2.10132
D68	-0.05100	-0.00025	0.00000	0.00034	0.00034	-0.05067
D69	3.13283	-0.00003	0.00000	-0.00118	-0.00118	3.13166
D70	-0.00756	0.00003	0.00000	0.00150	0.00150	-0.00606
D71	0.01878	-0.00012	0.00000	-0.00589	-0.00590	0.01288
D72	-3.12162	-0.00006	0.00000	-0.00322	-0.00322	-3.12484
D73	-0.97714	-0.00001	0.00000	0.00428	0.00429	-0.97285
D74	1.18676	-0.00011	0.00000	0.00013	0.00011	1.18688
D75	-2.99825	-0.00002	0.00000	0.00175	0.00171	-2.99655
D76	1.01335	-0.00013	0.00000	0.00283	0.00284	1.01619
D77	-3.10593	-0.00023	0.00000	-0.00132	-0.00133	-3.10726
D78	-1.00776	-0.00014	0.00000	0.00030	0.00026	-1.00750
D79	-3.10455	0.00022	0.00000	0.00756	0.00759	-3.09696
D80	-0.94064	0.00012	0.00000	0.00341	0.00341	-0.93723
D81	1.15752	0.00021	0.00000	0.00504	0.00500	1.16253
D82	0.03324	-0.00002	0.00000	0.01153	0.01151	0.04475
D83	-3.11478	-0.00032	0.00000	-0.03876	-0.03880	3.12960
D84	2.11019	-0.00001	0.00000	0.01345	0.01345	2.12364
D85	-1.03783	-0.00031	0.00000	-0.03684	-0.03687	-1.07469
D86	-2.07282	0.00015	0.00000	0.01581	0.01579	-2.05703
D87	1.06234	-0.00015	0.00000	-0.03448	-0.03452	1.02782
D88	-0.00777	0.00002	0.00000	0.00147	0.00147	-0.00630
D89	3.13673	0.00004	0.00000	0.00222	0.00222	3.13896
D90	3.13279	-0.00001	0.00000	0.00018	0.00018	3.13297

This journal is © The Royal Society of Chemistry 2014

```
   D91       -0.00589   0.00001   0.00000   0.00094   0.00094  -
0.00495
   D92       -3.13674  -0.00005   0.00000  -0.00233  -0.00233  -
3.13907
   D93        0.00930  -0.00003   0.00000  -0.00172  -0.00172
0.00758
   D94        0.00606   0.00001   0.00000   0.00035   0.00035
0.00640
   D95       -3.13110   0.00003   0.00000   0.00096   0.00095  -
3.13014
   D96       -0.00168   0.00001   0.00000   0.00025   0.00025  -
0.00144
   D97        3.13699  -0.00002   0.00000  -0.00051  -0.00051
3.13648
   D98       -3.13881   0.00002   0.00000   0.00086   0.00086  -
3.13796
   D99       -0.00014   0.00000   0.00000   0.00010   0.00010  -
0.00004
   D100      -3.13401   0.00001   0.00000   0.00068   0.00068  -
3.13332
   D101       0.00587  -0.00002   0.00000  -0.00046  -0.00046
0.00541
   D102       0.00210  -0.00001   0.00000  -0.00012  -0.00012
0.00198
   D103      -3.14121  -0.00004   0.00000  -0.00126  -0.00126
3.14071
   D104      -3.13960   0.00003   0.00000   0.00123   0.00123  -
3.13838
   D105      -0.00019   0.00001   0.00000   0.00030   0.00030
0.00010
   D106       0.00026   0.00000   0.00000   0.00008   0.00008
0.00035
   D107       3.13967  -0.00002   0.00000  -0.00085  -0.00084
3.13883
   D108      -0.00479   0.00001   0.00000   0.00024   0.00024  -
0.00456
   D109      -3.13945   0.00003   0.00000   0.00166   0.00166  -
3.13780
   D110       3.13463  -0.00001   0.00000  -0.00069  -0.00069
3.13394
   D111      -0.00003   0.00001   0.00000   0.00074   0.00074
0.00070
   D112       0.00859   0.00005   0.00000   0.01042   0.01039
0.01898
   D113      -3.12815  -0.00022   0.00000  -0.01711  -0.01705
3.13798
   D114      -0.02693  -0.00003   0.00000  -0.01400  -0.01398  -
0.04091
   D115       3.12056   0.00024   0.00000   0.03216   0.03201  -
3.13061
         Item               Value     Threshold  Converged?
 Maximum Force            0.002721     0.000450     NO
```

This journal is © The Royal Society of Chemistry 2014

```
 RMS     Force            0.000453     0.000300     NO
 Maximum Displacement     0.099853     0.001800     NO
 RMS     Displacement     0.013471     0.001200     NO
 Predicted change in Energy=-1.067355D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.656722   -1.063745   -0.024577
      2          6           0       -0.228112   -1.573461   -0.039744
      3          1           0       -0.161119   -2.662008    0.025116
      4          6           0       -1.757594    0.335955   -0.095926
      5          6           0        0.366953   -1.068692   -1.402583
      6          1           0       -0.177760   -1.542461   -2.224851
      7          6           0        0.528815   -0.873497    1.075716
      8          6           0        0.444343    0.529009    1.031059
      9          6           0       -0.386799    1.035242   -0.156612
     10          6           0        0.312271    0.470635   -1.467381
     11          1           0       -0.233934    0.841207   -2.339748
     12          6           0        1.270180   -1.493954    2.079526
     13          1           0        1.345216   -2.578271    2.111298
     14          6           0        1.092783    1.313213    1.981851
     15          1           0        1.031611    2.397075    1.937071
     16          6           0        1.828699    0.683696    2.993718
     17          1           0        2.336074    1.287094    3.741356
     18          6           0        1.917766   -0.709590    3.042147
     19          1           0        2.494832   -1.189419    3.828002
     20          6           0       -2.808754   -1.844219    0.034550
     21          1           0       -2.732283   -2.927876    0.089671
     22          6           0       -4.064355   -1.222074    0.030071
     23          1           0       -4.965868   -1.826543    0.083858
     24          6           0       -4.159847    0.169349   -0.039703
     25          1           0       -5.135275    0.648092   -0.039918
     26          6           0       -3.003232    0.958188   -0.106057
     27          1           0       -3.078828    2.040926   -0.156758
     28          6           0        1.842677   -1.406002   -1.553296
     29          6           0        1.775238    0.892181   -1.604073
     30          8           0        2.582711   -0.238451   -1.677101
     31          8           0        2.231270    1.993260   -1.701498
     32          8           0        2.358147   -2.486627   -1.594365
     33          6           0       -0.517869    2.493527   -0.196202
     34          7           0       -0.678131    3.642853   -0.207289
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  C    1.516894   0.000000
```

This journal is © The Royal Society of Chemistry 2014

3	H	2.189462	1.092534	0.000000		
4	C	1.405142	2.447109	3.398701	0.000000	
5	C	2.448303	1.570422	2.203598	2.862531	0.000000
6	H	2.694012	2.185907	2.513168	3.249099	1.094209
7	C	2.454263	1.518927	2.185987	2.839575	2.491238
8	C	2.840018	2.453404	3.400161	2.481107	2.912259
9	C	2.456804	2.616137	3.708587	1.540054	2.558735
10	C	2.883217	2.551174	3.502156	2.486639	1.541660
11	H	3.318612	3.334768	4.227340	2.758906	2.210668
12	C	3.630301	2.596634	2.762891	4.153140	3.622396
13	H	3.983388	2.848155	2.574532	4.794996	3.947556
14	C	4.151561	3.763575	4.604722	3.660170	4.201749
15	H	4.801299	4.610841	5.538276	4.020070	4.858663
16	C	4.930701	4.304315	4.895479	4.746401	4.953285
17	H	5.970855	5.390226	5.970076	5.691003	5.990599
18	C	4.723048	3.853455	4.151647	4.944587	4.721187
19	H	5.665118	4.745669	4.866676	5.983904	5.648139
20	C	1.392772	2.595870	2.771072	2.423864	3.570981
21	H	2.155196	2.849922	2.585680	3.411312	3.910070
22	C	2.413453	3.852935	4.160372	2.786481	4.659669
23	H	3.397656	4.746120	4.877199	3.873208	5.587739
24	C	2.790410	4.300689	4.900063	2.408679	4.886932
25	H	3.876977	5.386608	5.975218	3.392535	5.922729
26	C	2.430626	3.756985	4.604415	1.392441	4.140938
27	H	3.417431	4.604787	5.537480	2.157842	4.805747
28	C	3.834047	2.570418	2.843261	4.256794	1.521268
29	C	4.254269	3.541176	4.363025	3.881340	2.422579
30	O	4.624364	3.516236	4.037298	4.654923	2.382067
31	O	5.222434	4.640203	5.511464	4.608206	3.597301
32	O	4.539604	3.152690	3.000029	5.210721	2.451974
33	C	3.739067	4.080298	5.172600	2.490400	3.863634
34	N	4.810726	5.238370	6.330291	3.480405	4.971879

		6	7	8	9	10
6	H	0.000000				
7	C	3.441003	0.000000			
8	C	3.908829	1.405756	0.000000		
9	C	3.311475	2.449544	1.535458	0.000000	
10	C	2.206003	2.884601	2.502609	1.589212	0.000000
11	H	2.387097	3.897100	3.452517	2.197067	1.093933
12	C	4.541645	1.393637	2.423565	3.760681	4.166263
13	H	4.711109	2.155272	3.410818	4.604429	4.813496
14	C	5.240753	2.433278	1.392644	2.615235	3.635428
15	H	5.856972	3.419265	2.157641	2.872279	3.977300
16	C	6.017900	2.791645	2.406741	3.867375	4.716604
17	H	7.065505	3.878140	3.391024	4.761472	5.647417
18	C	5.729412	2.413069	2.783806	4.311324	4.930150
19	H	6.626040	3.397074	3.870451	5.397227	5.963257
20	C	3.481103	3.628456	4.148238	3.767454	4.165950
21	H	3.715101	3.978381	4.788237	4.611752	4.821161
22	C	4.504769	4.723568	4.939294	4.319114	4.925697
23	H	5.323234	5.664241	5.976303	5.405138	5.961722
24	C	4.854089	4.931049	4.740723	3.872897	4.704134

This journal is © The Royal Society of Chemistry 2014

25	H	5.843750	5.970074	5.682720	4.765662	5.634262
26	C	4.327335	4.150544	3.655544	2.618056	3.617109
27	H	5.053104	4.798743	4.013668	2.873747	3.960189
28	C	2.133488	2.986888	3.518309	3.589006	2.423074
29	C	3.182303	3.442739	2.974407	2.605765	1.528613
30	O	3.101721	3.492817	3.534932	3.571019	2.387820
31	O	4.310295	4.339304	3.578269	3.187280	2.460844
32	O	2.778450	3.616348	4.432782	4.690994	3.598212
33	C	4.529932	3.748356	2.508257	1.464698	2.529253
34	N	5.586449	4.847704	3.534046	2.624324	3.554110

		11	12	13	14	15
11	H	0.000000				
12	C	5.219705	0.000000			
13	H	5.830812	1.087375	0.000000		
14	C	4.545238	2.814462	3.901811	0.000000	
15	H	4.723719	3.900938	4.988263	1.086510	0.000000
16	C	5.720588	2.426902	3.413628	1.400620	2.165067
17	H	6.616916	3.410577	4.310445	2.154602	2.487794
18	C	5.999965	1.400440	2.164778	2.428282	3.414356
19	H	7.043490	2.156312	2.489498	3.411332	4.310403
20	C	4.413446	4.576277	4.701827	5.383619	6.029641
21	H	5.133207	4.694184	4.564559	6.016503	6.777528
22	C	4.954321	5.721141	5.952667	6.069037	6.534812
23	H	5.948274	6.556036	6.671236	7.082916	7.565918
24	C	4.599391	6.061593	6.517817	5.743277	5.985118
25	H	5.417533	7.078860	7.552080	6.581690	6.708049
26	C	3.559786	5.389975	6.027621	4.611155	4.746023
27	H	3.781295	6.034087	6.786252	4.744002	4.626735
28	C	3.159236	3.678707	3.879553	4.522581	5.225312
29	C	2.140231	4.417875	5.102248	3.674488	3.918850
30	O	3.088406	4.172682	4.621485	4.244465	4.734359
31	O	2.794963	5.232638	6.018422	3.914802	3.852458
32	O	4.283569	3.958099	3.842703	5.369288	6.171003
33	C	2.721318	4.927074	5.875268	2.954870	2.638380
34	N	3.548791	5.950817	6.940617	3.654544	3.012219

		16	17	18	19	20
16	C	0.000000				
17	H	1.086499	0.000000			
18	C	1.396970	2.156530	0.000000		
19	H	2.155998	2.483109	1.086651	0.000000	
20	C	6.054172	7.072113	5.716031	6.553401	0.000000
21	H	6.502268	7.535848	5.938085	6.657333	1.087749
22	C	6.866095	7.812493	6.717218	7.579465	1.401293
23	H	7.806070	8.740159	7.575188	8.371774	2.157750
24	C	6.732673	7.598865	6.870787	7.816019	2.425990
25	H	7.596127	8.398060	7.815869	8.749617	3.410258
26	C	5.747305	6.589306	6.075269	7.093501	2.812664
27	H	5.987603	6.714515	6.539440	7.574901	3.899217
28	C	5.004236	5.960667	4.648519	5.424996	4.934480
29	C	4.602826	5.389257	4.916639	5.861596	5.584438
30	O	4.820316	5.634518	4.789095	5.587327	5.880147
31	O	4.891020	5.489472	5.468624	6.385474	6.568253

This journal is © The Royal Society of Chemistry 2014

32	O	5.601944	6.535394	4.984881	5.577050	5.455539
33	C	4.354016	5.010472	5.165189	6.231748	4.910951
34	N	5.028643	5.497893	6.020073	7.049973	5.891180

		21	22	23	24	25
21	H	0.000000				
22	C	2.165116	0.000000			
23	H	2.490355	1.086739	0.000000		
24	C	3.412840	1.396440	2.156044	0.000000	
25	H	4.310302	2.156221	2.483513	1.086579	0.000000
26	C	3.900412	2.428591	3.412145	1.401580	2.155491
27	H	4.986964	3.413698	4.310004	2.164510	2.486486
28	C	5.093692	6.118326	7.015227	6.387722	7.429767
29	C	6.146490	6.421943	7.462110	6.180208	7.089524
30	O	6.213184	6.932925	7.912273	6.950501	7.939373
31	O	7.215450	7.278159	8.341294	6.850882	7.670483
32	O	5.379884	6.744362	7.542767	7.208011	8.270075
33	C	5.863187	5.141445	6.206943	4.323228	4.974987
34	N	6.890732	5.932147	6.955843	4.920941	5.372405

		26	27	28	29	30
26	C	0.000000				
27	H	1.086557	0.000000			
28	C	5.582717	6.168699	0.000000		
29	C	5.008212	5.193870	2.299733	0.000000	
30	O	5.924769	6.289676	1.387859	1.391285	0.000000
31	O	5.569274	5.530428	3.424610	1.195756	2.259345
32	O	6.544173	7.219844	1.197976	3.428735	2.260878
33	C	2.922743	2.600945	4.756071	3.131253	4.389802
34	N	3.552994	2.886532	5.801478	3.941601	5.278064

		31	32	33	34	
31	O	0.000000				
32	O	4.482964	0.000000			
33	C	3.173948	5.918468	0.000000		
34	N	3.663118	6.979505	1.160499	0.000000	

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.655642	-1.066185	-0.006955
2	6	0	-0.226176	-1.573525	0.007173
3	1	0	-0.158198	-2.659656	0.103754
4	6	0	-1.757905	0.330725	-0.119249
5	6	0	0.382217	-1.106740	-1.363300
6	1	0	-0.153217	-1.604755	-2.177292
7	6	0	0.518076	-0.840660	1.109959
8	6	0	0.431932	0.559845	1.024434

```
      9          6           0       -0.387622    1.030492   -0.185712
     10          6           0        0.325862    0.430011   -1.472553
     11          1           0       -0.211833    0.774561   -2.360729
     12          6           0        1.249939   -1.430891    2.138663
     13          1           0        1.326295   -2.513722    2.202133
     14          6           0        1.069282    1.372022    1.959106
     15          1           0        1.006924    2.454053    1.882790
     16          6           0        1.795625    0.772956    2.996064
     17          1           0        2.294300    1.398350    3.731377
     18          6           0        1.886311   -0.618218    3.085144
     19          1           0        2.455930   -1.074392    3.890284
     20          6           0       -2.807033   -1.846752    0.062524
     21          1           0       -2.729485   -2.928255    0.149329
     22          6           0       -4.063469   -1.227275    0.027336
     23          1           0       -4.964567   -1.831605    0.089041
     24          6           0       -4.160354    0.161417   -0.083092
     25          1           0       -5.136457    0.638181   -0.107034
     26          6           0       -3.004318    0.950147   -0.159986
     27          1           0       -3.081036    2.030859   -0.242337
     28          6           0        1.859937   -1.445523   -1.489088
     29          6           0        1.789523    0.850151   -1.606110
     30          8           0        2.599433   -0.280632   -1.638512
     31          8           0        2.244860    1.948832   -1.730200
     32          8           0        2.377453   -2.525940   -1.493984
     33          6           0       -0.520499    2.486814   -0.268246
     34          7           0       -0.682391    3.635062   -0.313775
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3748868      0.2675548
0.2564424
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1878.4290723852 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
```

This journal is © The Royal Society of Chemistry 2014

```
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1011.11146040     A.U. after   14 cycles
            Convg  =    0.8764D-08             -V/T =  2.0094
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000326320    0.000239492   -0.000015074
      2        6           0.000016855    0.000093262   -0.000085096
      3        1           0.000034757    0.000008565   -0.000016799
      4        6          -0.000405861   -0.000079895    0.000032663
      5        6           0.000416612   -0.000294085    0.001310434
      6        1           0.000129277   -0.000158431    0.000063139
      7        6           0.000080415    0.000085121   -0.000188546
      8        6           0.000117986   -0.000054522   -0.000173719
      9        6          -0.000012369   -0.000255340   -0.000125172
     10        6           0.000169233    0.000207374    0.002086933
     11        1           0.000355982    0.000204366   -0.000042179
     12        6          -0.000020436    0.000025319   -0.000039145
     13        1           0.000021682    0.000023509    0.000023809
     14        6          -0.000027091   -0.000072596   -0.000115754
     15        1           0.000034621   -0.000000901    0.000051704
     16        6          -0.000048810   -0.000040862   -0.000062028
     17        1          -0.000043400   -0.000019020   -0.000026846
     18        6          -0.000075037    0.000007438   -0.000047499
     19        1          -0.000044028    0.000020972   -0.000018159
     20        6           0.000065373    0.000078670    0.000026428
     21        1          -0.000019116    0.000042684   -0.000013771
     22        6           0.000058660    0.000038401    0.000001452
     23        1           0.000044090    0.000017291   -0.000011771
     24        6           0.000074639   -0.000047837   -0.000008892
     25        1           0.000060284    0.000005769   -0.000022148
     26        6           0.000143341   -0.000099640    0.000015588
     27        1          -0.000081943   -0.000051254   -0.000025358
     28        6          -0.000732629    0.000571599   -0.002723907
     29        6          -0.000948027    0.000062193   -0.004757997
     30        8           0.000325781   -0.000316326    0.002198138
     31        8           0.000242438    0.000232049    0.001770781
     32        8           0.000295423   -0.000370977    0.000960215
     33        6          -0.000031737   -0.000168751    0.000038316
     34        7           0.000129355    0.000066362   -0.000059737
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.004757997 RMS     0.000690179


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
```

This journal is © The Royal Society of Chemistry 2014

```
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000934899 RMS     0.000199736
 Search for a local minimum.
 Step number   2 out of a maximum of  204
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2
 DE= -1.16D-05 DEPred=-1.07D-04 R= 1.09D-01
 Trust test= 1.09D-01 RLast= 1.03D-01 DXMaxT set to 3.00D-01
     Eigenvalues ---    0.00426   0.00774   0.01069   0.01119
0.01164
     Eigenvalues ---    0.01421   0.01482   0.01578   0.01818
0.02009
     Eigenvalues ---    0.02114   0.02122   0.02128   0.02129
0.02130
     Eigenvalues ---    0.02131   0.02151   0.02158   0.02160
0.02162
     Eigenvalues ---    0.02169   0.02226   0.02966   0.03433
0.04219
     Eigenvalues ---    0.04771   0.04856   0.04942   0.05151
0.05293
     Eigenvalues ---    0.05534   0.06346   0.06526   0.07518
0.08540
     Eigenvalues ---    0.08756   0.09581   0.09971   0.12282
0.15848
     Eigenvalues ---    0.16000   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16001   0.16358   0.20218
0.20995
     Eigenvalues ---    0.22000   0.22001   0.22311   0.22615
0.22637
     Eigenvalues ---    0.24126   0.24586   0.24608   0.24768
0.24979
     Eigenvalues ---    0.26213   0.27340   0.27639   0.28721
0.28973
     Eigenvalues ---    0.29676   0.29960   0.34352   0.34404
0.34542
     Eigenvalues ---    0.35039   0.35156   0.35215   0.35242
0.35253
     Eigenvalues ---    0.35260   0.35267   0.35275   0.36434
0.37044
     Eigenvalues ---    0.40150   0.41706   0.42095   0.42137
0.43532
     Eigenvalues ---    0.44186   0.45508   0.46010   0.46123
0.46308
     Eigenvalues ---    0.46494   0.46522   0.46938   1.03901
1.07233
     Eigenvalues ---
1.275481000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     2    1
 RFO step:  Lambda=-4.49325803D-05.
 DIIS coeffs:      0.48778      0.51222
 Iteration  1 RMS(Cart)=  0.00519481 RMS(Int)=  0.00008075
 Iteration  2 RMS(Cart)=  0.00006579 RMS(Int)=  0.00004664
```

This journal is © The Royal Society of Chemistry 2014

```
 Iteration  3 RMS(Cart)=  0.00000001 RMS(Int)=  0.00004664
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86651   0.00018   0.00035  -0.00040  -0.00005
2.86646
    R2        2.65533  -0.00018  -0.00085   0.00187   0.00102
2.65635
    R3        2.63196  -0.00018  -0.00155   0.00364   0.00209
2.63404
    R4        2.06459  -0.00001  -0.00024   0.00059   0.00035
2.06494
    R5        2.96767  -0.00032  -0.00143   0.00301   0.00158
2.96925
    R6        2.87036  -0.00031  -0.00051   0.00066   0.00015
2.87051
    R7        2.91028   0.00020  -0.00102   0.00263   0.00161
2.91189
    R8        2.63133  -0.00018  -0.00162   0.00380   0.00217
2.63350
    R9        2.06775  -0.00004  -0.00042   0.00097   0.00055
2.06830
   R10        2.91331   0.00030  -0.00140   0.00393   0.00255
2.91586
   R11        2.87478  -0.00029   0.00019  -0.00087  -0.00071
2.87407
   R12        2.65649  -0.00021  -0.00088   0.00193   0.00104
2.65754
   R13        2.63359  -0.00012  -0.00145   0.00344   0.00199
2.63558
   R14        2.90159  -0.00026  -0.00086   0.00179   0.00093
2.90253
   R15        2.63172  -0.00015  -0.00142   0.00335   0.00192
2.63364
   R16        3.00318  -0.00039  -0.00256   0.00545   0.00290
3.00608
   R17        2.76788  -0.00011  -0.00061   0.00135   0.00074
2.76862
   R18        2.06723  -0.00007  -0.00042   0.00093   0.00051
2.06774
   R19        2.88866  -0.00027  -0.00106   0.00206   0.00103
2.88969
   R20        2.05484  -0.00002  -0.00052   0.00125   0.00073
2.05557
   R21        2.64645  -0.00015  -0.00163   0.00384   0.00221
2.64866
   R22        2.05321  -0.00001  -0.00049   0.00119   0.00070
2.05391
   R23        2.64679  -0.00012  -0.00156   0.00371   0.00215
2.64894
   R24        2.05318  -0.00005  -0.00039   0.00090   0.00051
2.05369
```

This journal is © The Royal Society of Chemistry 2014

R25	2.63989	-0.00010	-0.00161	0.00387	0.00226
2.64215					
R26	2.05347	-0.00005	-0.00039	0.00090	0.00051
2.05398					
R27	2.05555	-0.00004	-0.00051	0.00120	0.00069
2.05623					
R28	2.64806	-0.00015	-0.00179	0.00427	0.00248
2.65053					
R29	2.05364	-0.00005	-0.00037	0.00086	0.00048
2.05412					
R30	2.63889	-0.00012	-0.00154	0.00366	0.00212
2.64101					
R31	2.05334	-0.00005	-0.00037	0.00084	0.00047
2.05381					
R32	2.64860	-0.00013	-0.00181	0.00430	0.00249
2.65110					
R33	2.05330	-0.00005	-0.00042	0.00098	0.00056
2.05385					
R34	2.62267	-0.00013	-0.00008	0.00014	0.00003
2.62271					
R35	2.26385	0.00043	-0.00131	0.00341	0.00211
2.26595					
R36	2.62915	0.00025	-0.00089	0.00243	0.00156
2.63071					
R37	2.25965	0.00016	-0.00081	0.00207	0.00126
2.26091					
R38	2.19302	0.00005	-0.00023	0.00059	0.00036
2.19338					
A1	1.98431	0.00001	0.00000	0.00020	0.00019
1.98450					
A2	2.20326	-0.00006	0.00036	-0.00107	-0.00071
2.20255					
A3	2.09553	0.00005	-0.00037	0.00091	0.00054
2.09607					
A4	1.97355	0.00000	0.00121	-0.00285	-0.00163
1.97192					
A5	1.83127	0.00009	0.00182	-0.00344	-0.00162
1.82965					
A6	1.88298	0.00005	0.00080	-0.00165	-0.00085
1.88212					
A7	1.92680	-0.00002	-0.00128	0.00294	0.00166
1.92847					
A8	1.96600	0.00000	0.00004	-0.00026	-0.00022
1.96577					
A9	1.87586	-0.00011	-0.00265	0.00539	0.00275
1.87861					
A10	1.97187	-0.00010	-0.00027	0.00023	-0.00004
1.97183					
A11	2.10566	-0.00001	0.00040	-0.00090	-0.00050
2.10516					
A12	2.20565	0.00010	-0.00013	0.00068	0.00054
2.20619					

This journal is © The Royal Society of Chemistry 2014

A13	1.90111	-0.00010	0.00061	-0.00193	-0.00133
1.89978					
A14	1.92194	-0.00002	-0.00038	0.00066	0.00030
1.92224					
A15	1.96306	0.00010	-0.00252	0.00606	0.00354
1.96660					
A16	1.96393	0.00012	0.00077	-0.00063	0.00015
1.96408					
A17	1.88858	-0.00005	0.00193	-0.00496	-0.00301
1.88556					
A18	1.82517	-0.00004	-0.00047	0.00096	0.00046
1.82563					
A19	1.98940	0.00003	-0.00035	0.00073	0.00038
1.98978					
A20	2.20048	-0.00009	0.00038	-0.00099	-0.00061
2.19986					
A21	2.09327	0.00006	-0.00006	0.00032	0.00026
2.09353					
A22	1.96712	0.00003	0.00019	-0.00035	-0.00015
1.96697					
A23	2.10847	0.00001	0.00008	-0.00022	-0.00014
2.10832					
A24	2.20740	-0.00004	-0.00031	0.00069	0.00037
2.20777					
A25	1.87719	0.00006	0.00093	-0.00175	-0.00081
1.87638					
A26	1.83664	0.00016	0.00074	-0.00202	-0.00128
1.83536					
A27	1.95357	0.00003	0.00172	-0.00373	-0.00200
1.95156					
A28	1.85744	-0.00010	-0.00149	0.00365	0.00218
1.85962					
A29	1.97969	0.00000	-0.00036	0.00065	0.00028
1.97997					
A30	1.95065	-0.00015	-0.00155	0.00318	0.00163
1.95228					
A31	1.91312	-0.00009	0.00077	-0.00180	-0.00104
1.91207					
A32	1.97085	0.00018	0.00100	-0.00119	-0.00017
1.97068					
A33	1.81849	0.00003	0.00073	-0.00149	-0.00076
1.81772					
A34	1.89415	-0.00003	0.00061	-0.00185	-0.00124
1.89291					
A35	1.97880	0.00020	-0.00453	0.01221	0.00769
1.98648					
A36	1.88929	-0.00028	0.00131	-0.00559	-0.00428
1.88501					
A37	2.09637	0.00006	-0.00011	0.00043	0.00032
2.09669					
A38	2.08488	-0.00005	-0.00016	0.00025	0.00010
2.08497					

This journal is © The Royal Society of Chemistry 2014

A39	2.10193	-0.00001	0.00026	-0.00068	-0.00042
2.10152					
A40	2.10294	0.00008	-0.00059	0.00170	0.00110
2.10404					
A41	2.07691	-0.00004	-0.00027	0.00058	0.00031
2.07722					
A42	2.10333	-0.00005	0.00086	-0.00228	-0.00142
2.10191					
A43	2.08619	-0.00002	-0.00010	0.00019	0.00008
2.08627					
A44	2.10228	0.00003	0.00021	-0.00044	-0.00023
2.10205					
A45	2.09470	0.00000	-0.00011	0.00025	0.00014
2.09485					
A46	2.10052	-0.00001	0.00019	-0.00048	-0.00029
2.10023					
A47	2.08903	0.00000	-0.00015	0.00036	0.00022
2.08925					
A48	2.09362	0.00000	-0.00004	0.00011	0.00007
2.09369					
A49	2.09702	0.00003	-0.00022	0.00060	0.00038
2.09740					
A50	2.08544	-0.00002	-0.00007	0.00016	0.00009
2.08552					
A51	2.10072	0.00000	0.00030	-0.00077	-0.00047
2.10025					
A52	2.09001	0.00000	-0.00019	0.00044	0.00025
2.09026					
A53	2.09881	-0.00002	0.00026	-0.00066	-0.00040
2.09841					
A54	2.09436	0.00002	-0.00007	0.00022	0.00015
2.09451					
A55	2.09487	0.00002	-0.00006	0.00022	0.00016
2.09503					
A56	2.10219	0.00002	0.00016	-0.00036	-0.00020
2.10199					
A57	2.08612	-0.00004	-0.00010	0.00014	0.00004
2.08616					
A58	2.07873	-0.00002	-0.00038	0.00086	0.00048
2.07920					
A59	2.10351	0.00010	-0.00070	0.00202	0.00133
2.10484					
A60	2.10092	-0.00008	0.00108	-0.00289	-0.00181
2.09911					
A61	1.91725	0.00009	0.00004	0.00047	0.00027
1.91752					
A62	2.24057	-0.00002	-0.00113	0.00291	0.00166
2.24223					
A63	2.12511	-0.00004	0.00121	-0.00286	-0.00177
2.12334					
A64	1.91351	-0.00006	0.00009	0.00056	0.00034
1.91385					

This journal is © The Royal Society of Chemistry 2014

A65	2.24749	0.00009	-0.00127	0.00442	0.00282	2.25031
A66	2.12080	0.00004	0.00188	-0.00333	-0.00178	2.11902
A67	1.94927	0.00001	-0.00014	0.00043	0.00024	1.94951
A68	3.09199	0.00030	0.00188	-0.00161	0.00027	3.09226
A69	3.11569	0.00007	-0.00121	0.00362	0.00242	3.11811
D1	3.13262	-0.00002	0.00029	-0.00135	-0.00107	3.13155
D2	-1.04966	0.00002	0.00059	-0.00158	-0.00100	-1.05065
D3	0.94649	-0.00005	-0.00121	0.00220	0.00099	0.94749
D4	-0.02353	0.00000	-0.00078	0.00201	0.00123	-0.02230
D5	2.07738	0.00003	-0.00047	0.00178	0.00130	2.07868
D6	-2.20965	-0.00003	-0.00228	0.00556	0.00329	-2.20637
D7	-0.01195	0.00001	0.00117	-0.00180	-0.00063	-0.01258
D8	3.13000	0.00001	-0.00123	0.00315	0.00193	3.13193
D9	-3.13998	-0.00001	0.00216	-0.00491	-0.00276	3.14045
D10	0.00197	-0.00001	-0.00024	0.00004	-0.00020	0.00177
D11	0.01525	-0.00001	0.00067	-0.00221	-0.00154	0.01371
D12	-3.13262	-0.00001	0.00109	-0.00303	-0.00195	-3.13457
D13	3.14144	0.00000	-0.00045	0.00134	0.00089	-3.14086
D14	-0.00643	0.00001	-0.00004	0.00052	0.00048	-0.00595
D15	-1.11862	-0.00009	-0.00471	0.00734	0.00262	-1.11600
D16	1.04282	-0.00002	-0.00358	0.00569	0.00212	1.04494
D17	3.07096	-0.00003	-0.00594	0.01101	0.00506	3.07602
D18	1.01300	-0.00004	-0.00285	0.00345	0.00059	1.01359
D19	-3.10874	0.00003	-0.00172	0.00180	0.00009	-3.10865
D20	-1.08060	0.00002	-0.00408	0.00712	0.00303	-1.07757
D21	-3.11974	-0.00013	-0.00530	0.00846	0.00315	-3.11660

This journal is © The Royal Society of Chemistry 2014

D22	-0.95830	-0.00006	-0.00417	0.00681	0.00264	-0.95566
D23	1.06984	-0.00007	-0.00653	0.01214	0.00558	1.07542
D24	-0.93493	0.00001	0.00026	-0.00115	-0.00090	-0.93583
D25	2.21600	-0.00001	0.00350	-0.00894	-0.00544	2.21056
D26	-3.12555	-0.00002	-0.00192	0.00392	0.00199	-3.12356
D27	0.02538	-0.00004	0.00132	-0.00387	-0.00255	0.02283
D28	1.03145	0.00009	0.00146	-0.00331	-0.00185	1.02960
D29	-2.10081	0.00006	0.00470	-0.01109	-0.00639	-2.10720
D30	-0.93063	0.00005	-0.00029	0.00039	0.00010	-0.93053
D31	1.04457	0.00005	-0.00123	0.00285	0.00164	1.04621
D32	-3.11639	-0.00001	-0.00166	0.00332	0.00167	-3.11472
D33	2.21058	0.00005	0.00227	-0.00490	-0.00263	2.20794
D34	-2.09740	0.00004	0.00133	-0.00244	-0.00110	-2.09850
D35	0.02482	-0.00002	0.00090	-0.00197	-0.00107	0.02375
D36	0.00353	0.00000	0.00032	-0.00048	-0.00017	0.00336
D37	3.13675	0.00001	0.00105	-0.00187	-0.00082	3.13593
D38	-3.13765	0.00000	-0.00242	0.00518	0.00276	-3.13489
D39	-0.00443	0.00002	-0.00169	0.00379	0.00211	-0.00232
D40	-0.04203	0.00000	0.00374	-0.00513	-0.00140	-0.04343
D41	-2.15608	-0.00001	0.00173	-0.00069	0.00104	-2.15504
D42	2.08100	0.00021	-0.00079	0.00750	0.00670	2.08770
D43	2.08250	-0.00006	0.00479	-0.00757	-0.00278	2.07971
D44	-0.03156	-0.00007	0.00278	-0.00313	-0.00034	-0.03190
D45	-2.07766	0.00015	0.00026	0.00506	0.00532	-2.07234
D46	-2.15489	-0.00008	0.00720	-0.01323	-0.00603	-2.16092
D47	2.01424	-0.00009	0.00519	-0.00879	-0.00359	2.01065

This journal is © The Royal Society of Chemistry 2014

D48	-0.03187	0.00013	0.00267	-0.00060	0.00207	-0.02979
D49	-2.07521	0.00037	0.00338	0.01279	0.01615	-2.05906
D50	1.09088	-0.00058	-0.01185	-0.01131	-0.02318	1.06770
D51	2.10712	0.00046	0.00290	0.01475	0.01764	2.12476
D52	-1.00997	-0.00049	-0.01233	-0.00935	-0.02170	-1.03167
D53	0.01018	0.00037	0.00131	0.01741	0.01869	0.02888
D54	-3.10691	-0.00058	-0.01393	-0.00669	-0.02065	-3.12756
D55	-0.01281	0.00001	0.00080	-0.00062	0.00018	-0.01262
D56	-3.13451	-0.00001	0.00292	-0.00688	-0.00396	-3.13848
D57	3.12008	0.00004	-0.00222	0.00663	0.00442	3.12450
D58	-0.00162	0.00001	-0.00010	0.00037	0.00027	-0.00135
D59	0.00027	0.00002	-0.00322	0.00781	0.00459	0.00486
D60	3.13955	0.00003	-0.00256	0.00645	0.00389	-3.13974
D61	-3.13148	-0.00001	0.00020	-0.00040	-0.00020	-3.13168
D62	0.00780	0.00001	0.00086	-0.00176	-0.00090	0.00690
D63	0.94213	0.00000	-0.00058	0.00060	0.00002	0.94215
D64	-1.01903	-0.00016	-0.00115	0.00199	0.00083	-1.01820
D65	3.11217	0.00009	0.00208	-0.00504	-0.00296	3.10921
D66	-2.22071	0.00002	-0.00283	0.00727	0.00444	-2.21626
D67	2.10132	-0.00014	-0.00340	0.00866	0.00526	2.10657
D68	-0.05067	0.00012	-0.00017	0.00163	0.00146	-0.04921
D69	3.13166	0.00000	0.00060	-0.00119	-0.00059	3.13107
D70	-0.00606	-0.00002	-0.00077	0.00146	0.00069	-0.00537
D71	0.01288	-0.00002	0.00302	-0.00836	-0.00534	0.00754
D72	-3.12484	-0.00005	0.00165	-0.00571	-0.00406	-3.12890
D73	-0.97285	-0.00004	-0.00220	0.00237	0.00017	-0.97269

This journal is © The Royal Society of Chemistry 2014

D74	1.18688	0.00010	-0.00006	-0.00147	-0.00152	1.18535
D75	-2.99655	-0.00014	-0.00087	-0.00200	-0.00288	-2.99942
D76	1.01619	0.00006	-0.00146	0.00107	-0.00039	1.01581
D77	-3.10726	0.00020	0.00068	-0.00277	-0.00208	-3.10934
D78	-1.00750	-0.00004	-0.00013	-0.00330	-0.00343	-1.01093
D79	-3.09696	-0.00010	-0.00389	0.00638	0.00250	-3.09447
D80	-0.93723	0.00005	-0.00175	0.00254	0.00081	-0.93643
D81	1.16253	-0.00020	-0.00256	0.00202	-0.00054	1.16198
D82	0.04475	-0.00060	-0.00590	-0.01632	-0.02219	0.02256
D83	3.12960	0.00092	0.01988	0.01742	0.03737	-3.11621
D84	2.12364	-0.00059	-0.00689	-0.01298	-0.01985	2.10379
D85	-1.07469	0.00093	0.01888	0.02076	0.03971	-1.03499
D86	-2.05703	-0.00069	-0.00809	-0.01143	-0.01952	-2.07655
D87	1.02782	0.00083	0.01768	0.02231	0.04004	1.06786
D88	-0.00630	-0.00002	-0.00075	0.00132	0.00057	-0.00573
D89	3.13896	-0.00002	-0.00114	0.00234	0.00120	3.14016
D90	3.13297	0.00000	-0.00009	-0.00004	-0.00013	3.13284
D91	-0.00495	0.00000	-0.00048	0.00098	0.00050	-0.00446
D92	-3.13907	0.00002	0.00119	-0.00238	-0.00119	-3.14025
D93	0.00758	0.00001	0.00088	-0.00190	-0.00102	0.00655
D94	0.00640	0.00000	-0.00018	0.00026	0.00008	0.00649
D95	-3.13014	-0.00002	-0.00049	0.00074	0.00025	-3.12989
D96	-0.00144	0.00001	-0.00013	0.00052	0.00040	-0.00104
D97	3.13648	0.00001	0.00026	-0.00049	-0.00023	3.13625
D98	-3.13796	0.00000	-0.00044	0.00100	0.00057	-3.13739
D99	-0.00004	0.00000	-0.00005	-0.00001	-0.00007	-0.00010

This journal is © The Royal Society of Chemistry 2014

```
   D100      -3.13332  -0.00001  -0.00035   0.00061   0.00026  -
3.13306
   D101       0.00541   0.00000   0.00023  -0.00063  -0.00040
0.00501
   D102       0.00198   0.00000   0.00006  -0.00020  -0.00014
0.00184
   D103       3.14071   0.00001   0.00065  -0.00145  -0.00081
3.13991
   D104      -3.13838  -0.00001  -0.00063   0.00121   0.00058  -
3.13780
   D105       0.00010  -0.00001  -0.00015   0.00019   0.00003
0.00014
   D106       0.00035   0.00000  -0.00004  -0.00004  -0.00008
0.00026
   D107       3.13883   0.00000   0.00043  -0.00106  -0.00063
3.13820
   D108      -0.00456   0.00001  -0.00012   0.00037   0.00025  -
0.00431
   D109      -3.13780  -0.00001  -0.00085   0.00173   0.00088  -
3.13691
   D110       3.13394   0.00001   0.00035  -0.00065  -0.00030
3.13364
   D111       0.00070   0.00000  -0.00038   0.00072   0.00034
0.00104
   D112       0.01898  -0.00079  -0.00532  -0.02930  -0.03458  -
0.01561
   D113       3.13798   0.00009   0.00873  -0.00699   0.00165
3.13963
   D114      -0.04091   0.00088   0.00716   0.02881   0.03594  -
0.00497
   D115      -3.13061  -0.00052  -0.01639  -0.00233  -0.01852
3.13405
         Item               Value     Threshold  Converged?
 Maximum Force            0.000935     0.000450     NO
 RMS     Force            0.000200     0.000300     YES
 Maximum Displacement     0.038217     0.001800     NO
 RMS     Displacement     0.005192     0.001200     NO
 Predicted change in Energy=-1.352845D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                          Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.653586   -1.063242   -0.026592
      2          6           0       -0.224937   -1.572738   -0.042569
      3          1           0       -0.159467   -2.661472    0.023797
      4          6           0       -1.755029    0.336934   -0.098408
      5          6           0        0.366732   -1.068290   -1.407967
```

6	1	0	-0.182272	-1.541987	-2.227805
7	6	0	0.531264	-0.872611	1.073388
8	6	0	0.447063	0.530471	1.028953
9	6	0	-0.383712	1.037047	-0.159464
10	6	0	0.313470	0.472422	-1.473092
11	1	0	-0.236061	0.843246	-2.343601
12	6	0	1.268150	-1.494374	2.081144
13	1	0	1.342877	-2.579099	2.112950
14	6	0	1.091701	1.314611	1.983865
15	1	0	1.032014	2.398969	1.940067
16	6	0	1.824238	0.684310	2.999264
17	1	0	2.329219	1.287593	3.749001
18	6	0	1.912681	-0.710213	3.047677
19	1	0	2.486911	-1.190654	3.835604
20	6	0	-2.805749	-1.845200	0.036275
21	1	0	-2.728650	-2.929115	0.092589
22	6	0	-4.063084	-1.223590	0.034491
23	1	0	-4.964273	-1.828714	0.091416
24	6	0	-4.159496	0.168868	-0.035880
25	1	0	-5.135287	0.647431	-0.033485
26	6	0	-3.002183	0.958744	-0.105538
27	1	0	-3.080172	2.041628	-0.155788
28	6	0	1.840308	-1.408152	-1.569770
29	6	0	1.776453	0.890930	-1.624296
30	8	0	2.584528	-0.241478	-1.675636
31	8	0	2.240399	1.991627	-1.692450
32	8	0	2.358054	-2.489404	-1.595243
33	6	0	-0.518162	2.495469	-0.197159
34	7	0	-0.680843	3.644644	-0.208406

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.516865	0.000000			
3	H	2.188439	1.092717	0.000000		
4	C	1.405682	2.447682	3.398704	0.000000	
5	C	2.447428	1.571258	2.205688	2.862074	0.000000
6	H	2.690595	2.185869	2.514652	3.246266	1.094500
7	C	2.453542	1.519006	2.186041	2.839585	2.494491
8	C	2.840215	2.454227	3.400987	2.481453	2.915659
9	C	2.457936	2.617222	3.709840	1.540907	2.560150
10	C	2.884430	2.553226	3.505087	2.487328	1.543008
11	H	3.318524	3.336443	4.230069	2.757627	2.211955
12	C	3.628356	2.597230	2.762768	4.152559	3.628773
13	H	3.981740	2.849046	2.574565	4.794827	3.953765
14	C	4.151231	3.765203	4.606139	3.659998	4.208125
15	H	4.802822	4.613592	5.540738	4.021812	4.865574
16	C	4.930010	4.306522	4.897218	4.746303	4.961816
17	H	5.970281	5.392700	5.972086	5.690992	5.999655
18	C	4.721654	3.855253	4.152717	4.944336	4.729792
19	H	5.663612	4.747666	4.867905	5.983646	5.657310
20	C	1.393877	2.596352	2.769344	2.425668	3.571283

This journal is © The Royal Society of Chemistry 2014

21	H	2.156721	2.850719	2.584002	3.413428	3.910975
22	C	2.415601	3.854766	4.160029	2.789268	4.661338
23	H	3.400077	4.748135	4.876907	3.876250	5.589813
24	C	2.792449	4.302789	4.900471	2.411145	4.888755
25	H	3.879265	5.388949	5.975860	3.395110	5.924957
26	C	2.431743	3.758386	4.604750	1.393590	4.141832
27	H	3.419366	4.607476	5.539126	2.159926	4.808398
28	C	3.835056	2.573843	2.847694	4.258718	1.520892
29	C	4.258710	3.546419	4.368473	3.886722	2.423357
30	O	4.621283	3.511732	4.034099	4.653382	2.381992
31	O	5.222109	4.637315	5.509645	4.608950	3.599257
32	O	4.537384	3.150066	2.998134	5.210197	2.453569
33	C	3.739345	4.081689	5.174120	2.489751	3.866454
34	N	4.810767	5.239889	6.331891	3.479500	4.974747

		6	7	8	9	10
6	H	0.000000				
7	C	3.443120	0.000000			
8	C	3.911217	1.406308	0.000000		
9	C	3.312103	2.450286	1.535950	0.000000	
10	C	2.207531	2.888099	2.506282	1.590749	0.000000
11	H	2.388648	3.899843	3.455230	2.197684	1.094203
12	C	4.546761	1.394690	2.425136	3.762587	4.172804
13	H	4.716337	2.156734	3.412763	4.606678	4.819871
14	C	5.246077	2.434542	1.393661	2.616820	3.642180
15	H	5.863171	3.421274	2.159532	2.875264	3.984663
16	C	6.025341	2.793704	2.408817	3.870017	4.725388
17	H	7.073636	3.880467	3.393288	4.764333	5.656678
18	C	5.736845	2.415057	2.786140	4.314173	4.938973
19	H	6.634222	3.399344	3.873052	5.400342	5.972598
20	C	3.478596	3.627285	4.148495	3.769871	4.168824
21	H	3.713811	3.977212	4.788597	4.614402	4.824552
22	C	4.503339	4.723403	4.940356	4.322717	4.929857
23	H	5.322456	5.663863	5.977231	5.408980	5.966363
24	C	4.852821	4.931368	4.741837	3.876281	4.707988
25	H	5.843026	5.970385	5.683756	4.769186	5.638444
26	C	4.325456	4.150781	3.656199	2.620197	3.619430
27	H	5.053056	4.800639	4.016042	2.877515	3.964152
28	C	2.131138	2.997780	3.528846	3.593637	2.424281
29	C	3.181181	3.455152	2.989472	2.614077	1.529160
30	O	3.106670	3.488747	3.532628	3.569853	2.389222
31	O	4.317681	4.332997	3.571704	3.185471	2.463566
32	O	2.784060	3.615629	4.433727	4.691972	3.601064
33	C	4.531820	3.749606	2.509229	1.465091	2.532259
34	N	5.588174	4.849515	3.535719	2.624928	3.556836

		11	12	13	14	15
11	H	0.000000				
12	C	5.225465	0.000000			
13	H	5.836638	1.087761	0.000000		
14	C	4.551055	2.816202	3.903937	0.000000	
15	H	4.730549	3.903048	4.990760	1.086882	0.000000
16	C	5.728551	2.428753	3.415713	1.401758	2.165542
17	H	6.625550	3.412763	4.312869	2.155896	2.488000

This journal is © The Royal Society of Chemistry 2014

18	C	6.008012	1.401611	2.165900	2.430147	3.416049
19	H	7.052226	2.157719	2.490809	3.413488	4.312213
20	C	4.415297	4.571786	4.697051	5.382159	6.030408
21	H	5.136022	4.689055	4.558695	6.015082	6.778218
22	C	4.957140	5.717007	5.948261	6.067482	6.535608
23	H	5.951863	6.550871	6.665570	7.080726	7.566127
24	C	4.601490	6.058672	6.514975	5.741704	5.985774
25	H	5.420092	7.075521	7.548794	6.579530	6.708084
26	C	3.560014	5.388424	6.026406	4.610004	4.746946
27	H	3.783069	6.034491	6.786874	4.744596	4.629295
28	C	3.158942	3.696481	3.896277	4.538961	5.240845
29	C	2.137730	4.436027	5.118212	3.696920	3.941199
30	O	3.094920	4.173247	4.621640	4.247574	4.738730
31	O	2.806355	5.228526	6.014828	3.910645	3.849844
32	O	4.289060	3.961539	3.845689	5.374401	6.176810
33	C	2.723350	4.929546	5.878036	2.956848	2.641986
34	N	3.550313	5.954000	6.943998	3.657461	3.016873

		16	17	18	19	20
16	C	0.000000				
17	H	1.086766	0.000000			
18	C	1.398164	2.157913	0.000000		
19	H	2.157334	2.484768	1.086919	0.000000	
20	C	6.050993	7.068707	5.711420	6.547945	0.000000
21	H	6.498799	7.532065	5.932791	6.650900	1.088111
22	C	6.862254	7.808019	6.712124	7.573109	1.402602
23	H	7.800946	8.734090	7.568555	8.363385	2.159291
24	C	6.729254	7.594754	6.866763	7.810980	2.427820
25	H	7.591700	8.392607	7.810929	8.743358	3.412451
26	C	5.745386	6.587068	6.073226	7.091027	2.814391
27	H	5.987479	6.713975	6.539373	7.574382	3.901235
28	C	5.025408	5.982926	4.670457	5.448253	4.935204
29	C	4.628421	5.416199	4.940602	5.886276	5.589319
30	O	4.825952	5.641802	4.793827	5.593230	5.878576
31	O	4.888195	5.487527	5.465908	6.383342	6.570643
32	O	5.609538	6.544271	4.992052	5.585468	5.453596
33	C	4.357092	5.013853	5.168593	6.235474	4.912123
34	N	5.032709	5.502476	6.024386	7.054700	5.891815

		21	22	23	24	25
21	H	0.000000				
22	C	2.166311	0.000000			
23	H	2.491766	1.086995	0.000000		
24	C	3.414868	1.397565	2.157360	0.000000	
25	H	4.312711	2.157535	2.485184	1.086828	0.000000
26	C	3.902501	2.430576	3.414455	1.402900	2.156905
27	H	4.989343	3.415256	4.311670	2.164844	2.486412
28	C	5.094324	6.120274	7.017032	6.390419	7.432665
29	C	6.151129	6.428294	7.468435	6.187078	7.096628
30	O	6.211270	6.933962	7.913672	6.952629	7.942441
31	O	7.217445	7.283807	8.347723	6.857502	7.678527
32	O	5.377423	6.744578	7.543064	7.209472	8.272181
33	C	5.864837	5.143105	6.208843	4.324164	4.975929
34	N	6.891909	5.932812	6.956674	4.920550	5.371774

		26	27	28	29	30
26	C	0.000000				
27	H	1.086852	0.000000			
28	C	5.585328	6.173447	0.000000		
29	C	5.014638	5.202637	2.300615	0.000000	
30	O	5.925967	6.293754	1.387877	1.392109	0.000000
31	O	5.574030	5.538258	3.425438	1.196421	2.259527
32	O	6.545310	7.223336	1.199090	3.430126	2.260736
33	C	2.922376	2.602225	4.762845	3.142694	4.393570
34	N	3.551516	2.886036	5.808637	3.952972	5.283688

		31	32	33	34
31	O	0.000000			
32	O	4.483629	0.000000		
33	C	3.177957	5.922518	0.000000	
34	N	3.669946	6.984609	1.160688	0.000000

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.652745	-1.066339	-0.003620
2	6	0	-0.223064	-1.572778	0.016622
3	1	0	-0.156408	-2.658253	0.123069
4	6	0	-1.755882	0.330096	-0.127209
5	6	0	0.384743	-1.116562	-1.358620
6	1	0	-0.153055	-1.620801	-2.167598
7	6	0	0.517780	-0.831093	1.115909
8	6	0	0.431535	0.569273	1.019791
9	6	0	-0.385211	1.030716	-0.196408
10	6	0	0.329438	0.420670	-1.479998
11	1	0	-0.209822	0.758570	-2.370112
12	6	0	1.243125	-1.414382	2.154566
13	1	0	1.319463	-2.497078	2.226451
14	6	0	1.062689	1.388848	1.953725
15	1	0	1.001540	2.470778	1.870058
16	6	0	1.783605	0.797291	3.000275
17	1	0	2.278021	1.428400	3.733975
18	6	0	1.874025	-0.594369	3.100112
19	1	0	2.439221	-1.044737	3.911970
20	6	0	-2.804151	-1.848179	0.073076
21	1	0	-2.725749	-2.929174	0.169451
22	6	0	-4.062518	-1.229944	0.033174
23	1	0	-4.963224	-1.834700	0.100674
24	6	0	-4.160628	0.158842	-0.088630
25	1	0	-5.137260	0.634924	-0.115681
26	6	0	-3.004003	0.948361	-0.172334

```
     27          1           0       -3.083367    2.028544   -0.262623
     28          6           0        1.860861   -1.458636   -1.489664
     29          6           0        1.793422    0.836828   -1.627967
     30          8           0        2.604181   -0.294825   -1.628305
     31          8           0        2.256139    1.935417   -1.730035
     32          8           0        2.380895   -2.538904   -1.469620
     33          6           0       -0.521889    2.486513   -0.288416
     34          7           0       -0.686551    3.634156   -0.343180
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3740852      0.2672996
0.2563908
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1877.3386213740 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1011.11147413     A.U. after   14 cycles
             Convg  =    0.4144D-08             -V/T =  2.0094
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.001214045    0.000231702    0.000082332
      2        6           0.000309053    0.000080308   -0.000193926
      3        1           0.000212507    0.000161391   -0.000192249
      4        6          -0.001074308   -0.000234042    0.000068332
      5        6           0.000069204   -0.000374434   -0.000635979
      6        1          -0.000231573    0.000089368    0.000287608
      7        6           0.000506036    0.000177194    0.000428795
```

8	6	0.000387301	-0.000073110	0.000329601
9	6	0.000462306	-0.000061887	-0.000185946
10	6	-0.000072559	-0.000049056	-0.000568205
11	1	-0.000203816	-0.000119013	0.000207119
12	6	0.000130250	0.000798766	-0.000021736
13	1	-0.000036534	0.000307415	-0.000014774
14	6	0.000275740	-0.000696404	-0.000037557
15	1	-0.000073112	-0.000284768	-0.000037239
16	6	-0.000476748	-0.000680550	-0.000741918
17	1	-0.000162269	-0.000131561	-0.000162939
18	6	-0.000531021	0.000469153	-0.000770324
19	1	-0.000182585	0.000097891	-0.000156949
20	6	-0.000219859	0.000913713	-0.000055526
21	1	0.000013948	0.000316598	-0.000044329
22	6	0.000954392	0.000543562	-0.000024003
23	1	0.000221460	0.000114817	-0.000030255
24	6	0.001066493	-0.000499300	-0.000012006
25	1	0.000249899	-0.000067292	-0.000031330
26	6	-0.000051971	-0.000833058	0.000032982
27	1	0.000110544	-0.000261168	-0.000036446
28	6	0.001092877	-0.000464339	0.002294953
29	6	0.000587721	0.000844566	0.003237643
30	8	-0.000658149	-0.000108247	-0.001326051
31	8	-0.000910193	-0.000881828	-0.000851241
32	8	-0.000978855	0.001058922	-0.000633314
33	6	0.000255250	0.000008064	-0.000193296
34	7	0.000172616	-0.000393371	-0.000011828

Cartesian Forces: Max 0.003237643 RMS 0.000618304

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal Forces: Max 0.001508468 RMS 0.000387152
Search for a local minimum.
Step number 3 out of a maximum of 204
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swaping is turned off.
Update second derivatives using D2CorX and points 1 2 3
DE= -1.37D-05 DEPred=-1.35D-04 R= 1.01D-01
Trust test= 1.01D-01 RLast= 1.09D-01 DXMaxT set to 3.00D-01
Eigenvalues --- 0.00432 0.00769 0.01040 0.01147
0.01165
Eigenvalues --- 0.01423 0.01483 0.01577 0.01821
0.02114
Eigenvalues --- 0.02119 0.02128 0.02129 0.02130
0.02130
Eigenvalues --- 0.02150 0.02151 0.02155 0.02160
0.02162

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.02169   0.02772   0.03227   0.03812
0.04254
     Eigenvalues ---    0.04761   0.04854   0.04944   0.05311
0.05395
     Eigenvalues ---    0.05532   0.06450   0.06612   0.07623
0.08546
     Eigenvalues ---    0.08734   0.09760   0.10082   0.12290
0.15821
     Eigenvalues ---    0.15999   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16004   0.16391   0.20401
0.21597
     Eigenvalues ---    0.22000   0.22005   0.22349   0.22616
0.22664
     Eigenvalues ---    0.24371   0.24592   0.24723   0.24792
0.25000
     Eigenvalues ---    0.26419   0.27312   0.27767   0.28779
0.29037
     Eigenvalues ---    0.29742   0.30212   0.34366   0.34404
0.34554
     Eigenvalues ---    0.35144   0.35184   0.35241   0.35252
0.35260
     Eigenvalues ---    0.35267   0.35273   0.35351   0.36506
0.37037
     Eigenvalues ---    0.40129   0.42098   0.42137   0.43417
0.44127
     Eigenvalues ---    0.44813   0.45745   0.46012   0.46148
0.46481
     Eigenvalues ---    0.46521   0.46934   0.49321   1.03705
1.07323
     Eigenvalues ---
1.275821000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     3    2    1
 RFO step:  Lambda=-6.28986518D-05.
 DIIS coeffs:      0.39037      0.30349      0.30614
 Iteration  1 RMS(Cart)=  0.00578578 RMS(Int)=  0.00001886
 Iteration  2 RMS(Cart)=  0.00001833 RMS(Int)=  0.00001347
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00001347
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86646   0.00016   0.00024   0.00048   0.00073
2.86719
    R2        2.65635  -0.00070  -0.00113  -0.00020  -0.00133
2.65503
    R3        2.63404  -0.00131  -0.00220  -0.00009  -0.00229
2.63176
    R4        2.06494  -0.00016  -0.00036  -0.00002  -0.00037
2.06456
    R5        2.96925  -0.00101  -0.00182  -0.00074  -0.00255
2.96669
    R6        2.87051  -0.00041  -0.00040  -0.00065  -0.00105
2.86946
    R7        2.91189  -0.00008  -0.00159   0.00035  -0.00124
2.91065
```

This journal is © The Royal Society of Chemistry 2014

R8	2.63350	-0.00137	-0.00230	-0.00013	-0.00242
2.63108					
R9	2.06830	-0.00014	-0.00058	0.00010	-0.00049
2.06782					
R10	2.91586	-0.00065	-0.00239	0.00068	-0.00171
2.91415					
R11	2.87407	-0.00044	0.00055	-0.00085	-0.00028
2.87379					
R12	2.65754	-0.00078	-0.00116	-0.00021	-0.00137
2.65617					
R13	2.63558	-0.00119	-0.00208	-0.00006	-0.00214
2.63344					
R14	2.90253	-0.00066	-0.00108	-0.00039	-0.00147
2.90106					
R15	2.63364	-0.00126	-0.00202	-0.00014	-0.00216
2.63147					
R16	3.00608	-0.00151	-0.00330	-0.00113	-0.00444
3.00165					
R17	2.76862	-0.00042	-0.00082	-0.00011	-0.00093
2.76769					
R18	2.06774	-0.00010	-0.00056	0.00011	-0.00045
2.06729					
R19	2.88969	-0.00082	-0.00126	-0.00070	-0.00198
2.88772					
R20	2.05557	-0.00031	-0.00076	0.00000	-0.00075
2.05482					
R21	2.64866	-0.00127	-0.00232	-0.00006	-0.00238
2.64628					
R22	2.05391	-0.00028	-0.00072	0.00003	-0.00069
2.05322					
R23	2.64894	-0.00120	-0.00224	-0.00002	-0.00226
2.64668					
R24	2.05369	-0.00026	-0.00054	-0.00006	-0.00060
2.05309					
R25	2.64215	-0.00118	-0.00234	0.00006	-0.00228
2.63986					
R26	2.05398	-0.00025	-0.00054	-0.00005	-0.00059
2.05339					
R27	2.05623	-0.00032	-0.00072	-0.00003	-0.00075
2.05548					
R28	2.65053	-0.00136	-0.00258	0.00000	-0.00258
2.64796					
R29	2.05412	-0.00025	-0.00052	-0.00005	-0.00057
2.05355					
R30	2.64101	-0.00114	-0.00221	0.00002	-0.00220
2.63882					
R31	2.05381	-0.00025	-0.00051	-0.00007	-0.00058
2.05323					
R32	2.65110	-0.00133	-0.00260	0.00002	-0.00258
2.64851					
R33	2.05385	-0.00027	-0.00059	-0.00004	-0.00063
2.05322					

This journal is © The Royal Society of Chemistry 2014

R34	2.62271	-0.00020	-0.00007	-0.00020	-0.00025
2.62245					
R35	2.26595	-0.00137	-0.00206	0.00053	-0.00153
2.26442					
R36	2.63071	-0.00015	-0.00148	0.00055	-0.00093
2.62977					
R37	2.26091	-0.00111	-0.00125	0.00021	-0.00104
2.25987					
R38	2.19338	-0.00041	-0.00036	0.00005	-0.00031
2.19307					
A1	1.98450	-0.00010	-0.00012	0.00029	0.00018
1.98468					
A2	2.20255	0.00013	0.00064	-0.00041	0.00023
2.20278					
A3	2.09607	-0.00002	-0.00055	0.00013	-0.00043
2.09564					
A4	1.97192	0.00014	0.00172	0.00014	0.00186
1.97378					
A5	1.82965	0.00006	0.00208	-0.00012	0.00196
1.83161					
A6	1.88212	0.00010	0.00100	0.00013	0.00113
1.88325					
A7	1.92847	0.00000	-0.00178	0.00000	-0.00178
1.92669					
A8	1.96577	0.00007	0.00016	0.00006	0.00022
1.96599					
A9	1.87861	-0.00039	-0.00326	-0.00024	-0.00350
1.87511					
A10	1.97183	0.00002	-0.00014	-0.00033	-0.00047
1.97136					
A11	2.10516	0.00005	0.00055	0.00003	0.00058
2.10573					
A12	2.20619	-0.00007	-0.00041	0.00030	-0.00010
2.20609					
A13	1.89978	0.00007	0.00118	-0.00086	0.00031
1.90010					
A14	1.92224	0.00000	-0.00040	-0.00015	-0.00055
1.92168					
A15	1.96660	-0.00030	-0.00367	0.00084	-0.00283
1.96377					
A16	1.96408	-0.00009	0.00037	0.00033	0.00070
1.96478					
A17	1.88556	0.00032	0.00299	0.00013	0.00311
1.88868					
A18	1.82563	-0.00001	-0.00056	-0.00022	-0.00077
1.82486					
A19	1.98978	0.00004	-0.00044	0.00008	-0.00036
1.98943					
A20	2.19986	-0.00003	0.00060	-0.00029	0.00031
2.20018					
A21	2.09353	-0.00001	-0.00020	0.00022	0.00002
2.09355					

This journal is © The Royal Society of Chemistry 2014

A22	1.96697	0.00008	0.00021	0.00016	0.00037
1.96734					
A23	2.10832	0.00005	0.00013	-0.00002	0.00011
2.10843					
A24	2.20777	-0.00012	-0.00041	-0.00012	-0.00053
2.20725					
A25	1.87638	0.00017	0.00105	0.00048	0.00153
1.87791					
A26	1.83536	0.00006	0.00122	-0.00046	0.00076
1.83612					
A27	1.95156	0.00019	0.00225	0.00052	0.00277
1.95433					
A28	1.85962	-0.00029	-0.00222	-0.00003	-0.00224
1.85737					
A29	1.97997	0.00005	-0.00039	-0.00006	-0.00045
1.97953					
A30	1.95228	-0.00019	-0.00192	-0.00047	-0.00238
1.94991					
A31	1.91207	0.00022	0.00110	0.00016	0.00127
1.91334					
A32	1.97068	-0.00013	0.00070	0.00015	0.00086
1.97154					
A33	1.81772	0.00023	0.00090	0.00023	0.00114
1.81886					
A34	1.89291	0.00007	0.00112	-0.00029	0.00083
1.89374					
A35	1.98648	-0.00070	-0.00739	0.00054	-0.00685
1.97963					
A36	1.88501	0.00030	0.00339	-0.00077	0.00262
1.88763					
A37	2.09669	0.00003	-0.00026	0.00024	-0.00002
2.09667					
A38	2.08497	-0.00010	-0.00015	-0.00016	-0.00031
2.08466					
A39	2.10152	0.00006	0.00041	-0.00007	0.00034
2.10185					
A40	2.10404	-0.00002	-0.00103	0.00046	-0.00057
2.10347					
A41	2.07722	-0.00014	-0.00035	-0.00009	-0.00044
2.07678					
A42	2.10191	0.00016	0.00138	-0.00036	0.00102
2.10293					
A43	2.08627	-0.00008	-0.00011	-0.00011	-0.00022
2.08605					
A44	2.10205	0.00012	0.00026	0.00009	0.00036
2.10241					
A45	2.09485	-0.00005	-0.00015	0.00001	-0.00014
2.09471					
A46	2.10023	0.00008	0.00029	-0.00004	0.00025
2.10048					
A47	2.08925	-0.00006	-0.00022	0.00002	-0.00020
2.08905					

This journal is © The Royal Society of Chemistry 2014

A48	2.09369	-0.00003	-0.00007	0.00002	-0.00005	2.09365
A49	2.09740	0.00001	-0.00036	0.00015	-0.00021	2.09718
A50	2.08552	-0.00010	-0.00010	-0.00007	-0.00017	2.08536
A51	2.10025	0.00009	0.00046	-0.00008	0.00039	2.10063
A52	2.09026	-0.00007	-0.00026	-0.00002	-0.00029	2.08997
A53	2.09841	0.00009	0.00040	-0.00007	0.00033	2.09874
A54	2.09451	-0.00001	-0.00014	0.00009	-0.00004	2.09447
A55	2.09503	-0.00002	-0.00013	0.00013	0.00000	2.09502
A56	2.10199	0.00014	0.00022	0.00008	0.00029	2.10228
A57	2.08616	-0.00012	-0.00008	-0.00020	-0.00029	2.08587
A58	2.07920	-0.00015	-0.00052	-0.00009	-0.00060	2.07860
A59	2.10484	-0.00002	-0.00123	0.00061	-0.00062	2.10422
A60	2.09911	0.00017	0.00175	-0.00052	0.00123	2.10034
A61	1.91752	-0.00008	-0.00014	0.00028	0.00020	1.91771
A62	2.24223	-0.00034	-0.00169	0.00011	-0.00158	2.24065
A63	2.12334	0.00043	0.00180	-0.00033	0.00147	2.12481
A64	1.91385	-0.00009	-0.00015	-0.00026	-0.00032	1.91353
A65	2.25031	-0.00043	-0.00248	0.00051	-0.00185	2.24846
A66	2.11902	0.00053	0.00221	-0.00026	0.00207	2.12109
A67	1.94951	-0.00004	-0.00023	-0.00001	-0.00023	1.94928
A68	3.09226	0.00025	0.00096	0.00261	0.00357	3.09583
A69	3.11811	0.00001	-0.00220	0.00133	-0.00087	3.11724
D1	3.13155	0.00008	0.00082	0.00005	0.00087	3.13243
D2	-1.05065	0.00019	0.00096	0.00005	0.00101	-1.04964
D3	0.94749	-0.00018	-0.00133	-0.00022	-0.00155	0.94594
D4	-0.02230	0.00004	-0.00121	0.00043	-0.00078	-0.02308

This journal is © The Royal Society of Chemistry 2014

D5	2.07868	0.00015	-0.00108	0.00043	-0.00065	2.07803
D6	-2.20637	-0.00022	-0.00337	0.00016	-0.00321	-2.20957
D7	-0.01258	0.00000	0.00108	-0.00011	0.00097	-0.01161
D8	3.13193	-0.00006	-0.00191	-0.00022	-0.00213	3.12980
D9	3.14045	0.00004	0.00297	-0.00046	0.00251	-3.14023
D10	0.00177	-0.00002	-0.00002	-0.00057	-0.00059	0.00119
D11	0.01371	0.00003	0.00134	-0.00036	0.00098	0.01469
D12	-3.13457	0.00005	0.00184	-0.00010	0.00174	-3.13283
D13	-3.14086	-0.00002	-0.00081	0.00004	-0.00077	3.14156
D14	-0.00595	0.00000	-0.00031	0.00030	-0.00001	-0.00596
D15	-1.11600	-0.00007	-0.00441	-0.00050	-0.00491	-1.12091
D16	1.04494	-0.00014	-0.00343	-0.00075	-0.00419	1.04075
D17	3.07602	-0.00033	-0.00663	-0.00061	-0.00724	3.06878
D18	1.01359	0.00013	-0.00207	-0.00040	-0.00246	1.01113
D19	-3.10865	0.00006	-0.00108	-0.00066	-0.00174	-3.11039
D20	-1.07757	-0.00013	-0.00428	-0.00051	-0.00479	-1.08237
D21	-3.11660	-0.00005	-0.00509	-0.00049	-0.00558	-3.12218
D22	-0.95566	-0.00011	-0.00411	-0.00075	-0.00486	-0.96052
D23	1.07542	-0.00031	-0.00731	-0.00060	-0.00791	1.06751
D24	-0.93583	0.00009	0.00070	0.00012	0.00083	-0.93500
D25	2.21056	0.00015	0.00541	-0.00087	0.00454	2.21510
D26	-3.12356	-0.00020	-0.00236	-0.00019	-0.00255	-3.12611
D27	0.02283	-0.00015	0.00235	-0.00119	0.00116	0.02399
D28	1.02960	0.00003	0.00200	-0.00006	0.00194	1.03154
D29	-2.10720	0.00009	0.00671	-0.00105	0.00566	-2.10155
D30	-0.93053	0.00013	-0.00023	0.00053	0.00030	-0.93024

This journal is © The Royal Society of Chemistry 2014

D31	1.04621	-0.00010	-0.00173	0.00049	-0.00124	1.04497
D32	-3.11472	-0.00018	-0.00201	-0.00008	-0.00209	-3.11681
D33	2.20794	0.00019	0.00296	0.00064	0.00361	2.21155
D34	-2.09850	-0.00004	0.00147	0.00060	0.00207	-2.09643
D35	0.02375	-0.00012	0.00119	0.00004	0.00123	0.02498
D36	0.00336	0.00002	0.00029	0.00039	0.00068	0.00405
D37	3.13593	0.00005	0.00113	0.00064	0.00177	3.13771
D38	-3.13489	-0.00004	-0.00313	0.00027	-0.00286	-3.13775
D39	-0.00232	-0.00002	-0.00229	0.00052	-0.00177	-0.00409
D40	-0.04343	0.00009	0.00309	0.00103	0.00412	-0.03931
D41	-2.15504	-0.00007	0.00040	0.00119	0.00158	-2.15346
D42	2.08770	-0.00049	-0.00456	0.00189	-0.00267	2.08503
D43	2.07971	0.00012	0.00456	0.00005	0.00460	2.08432
D44	-0.03190	-0.00004	0.00187	0.00021	0.00207	-0.02982
D45	-2.07234	-0.00046	-0.00309	0.00091	-0.00218	-2.07452
D46	-2.16092	0.00045	0.00798	0.00024	0.00822	-2.15270
D47	2.01065	0.00029	0.00529	0.00040	0.00569	2.01634
D48	-0.02979	-0.00013	0.00033	0.00110	0.00143	-0.02836
D49	-2.05906	-0.00005	-0.00783	0.00024	-0.00758	-2.06664
D50	1.06770	0.00052	0.00705	0.00489	0.01195	1.07964
D51	2.12476	-0.00018	-0.00902	0.00071	-0.00831	2.11645
D52	-1.03167	0.00039	0.00586	0.00536	0.01122	-1.02045
D53	0.02888	-0.00022	-0.01061	0.00037	-0.01024	0.01863
D54	-3.12756	0.00035	0.00426	0.00502	0.00928	-3.11827
D55	-0.01262	0.00002	0.00037	0.00039	0.00077	-0.01186
D56	-3.13848	0.00007	0.00416	-0.00059	0.00357	-3.13490

This journal is © The Royal Society of Chemistry 2014

D57	3.12450	-0.00003	-0.00402	0.00132	-0.00270	3.12180
D58	-0.00135	0.00001	-0.00023	0.00033	0.00011	-0.00125
D59	0.00486	-0.00005	-0.00472	0.00116	-0.00357	0.00130
D60	-3.13974	-0.00003	-0.00390	0.00142	-0.00248	3.14096
D61	-3.13168	0.00001	0.00024	0.00011	0.00035	-3.13133
D62	0.00690	0.00003	0.00106	0.00038	0.00144	0.00834
D63	0.94215	-0.00009	-0.00036	-0.00045	-0.00081	0.94134
D64	-1.01820	-0.00010	-0.00120	-0.00013	-0.00133	-1.01952
D65	3.10921	0.00031	0.00305	0.00052	0.00357	3.11277
D66	-2.21626	-0.00014	-0.00440	0.00060	-0.00380	-2.22007
D67	2.10657	-0.00015	-0.00524	0.00092	-0.00432	2.10226
D68	-0.04921	0.00026	-0.00099	0.00157	0.00058	-0.04863
D69	3.13107	0.00000	0.00072	-0.00023	0.00049	3.13156
D70	-0.00537	-0.00005	-0.00088	-0.00075	-0.00163	-0.00700
D71	0.00754	0.00006	0.00506	-0.00136	0.00370	0.01124
D72	-3.12890	0.00000	0.00346	-0.00188	0.00158	-3.12732
D73	-0.97269	-0.00004	-0.00141	-0.00116	-0.00257	-0.97526
D74	1.18535	-0.00002	0.00089	-0.00105	-0.00016	1.18520
D75	-2.99942	-0.00004	0.00123	-0.00189	-0.00065	-3.00007
D76	1.01581	0.00005	-0.00064	-0.00083	-0.00147	1.01434
D77	-3.10934	0.00007	0.00167	-0.00073	0.00094	-3.10840
D78	-1.01093	0.00005	0.00201	-0.00157	0.00045	-1.01048
D79	-3.09447	-0.00020	-0.00384	-0.00123	-0.00508	-3.09955
D80	-0.93643	-0.00018	-0.00154	-0.00113	-0.00266	-0.93909
D81	1.16198	-0.00020	-0.00120	-0.00196	-0.00316	1.15882
D82	0.02256	0.00043	0.01000	-0.00228	0.00772	0.03028

This journal is © The Royal Society of Chemistry 2014

D83	-3.11621	-0.00047	-0.01090	-0.00028	-0.01119	-3.12740
D84	2.10379	0.00047	0.00799	-0.00164	0.00634	2.11012
D85	-1.03499	-0.00043	-0.01292	0.00036	-0.01258	-1.04756
D86	-2.07655	0.00033	0.00707	-0.00221	0.00486	-2.07169
D87	1.06786	-0.00058	-0.01384	-0.00021	-0.01405	1.05381
D88	-0.00573	-0.00004	-0.00080	-0.00066	-0.00146	-0.00719
D89	3.14016	-0.00005	-0.00141	-0.00050	-0.00191	3.13825
D90	3.13284	-0.00002	0.00003	-0.00040	-0.00037	3.13247
D91	-0.00446	-0.00002	-0.00059	-0.00023	-0.00082	-0.00528
D92	-3.14025	0.00006	0.00144	0.00059	0.00202	-3.13823
D93	0.00655	0.00005	0.00115	0.00046	0.00161	0.00816
D94	0.00649	0.00000	-0.00016	0.00007	-0.00008	0.00640
D95	-3.12989	-0.00001	-0.00044	-0.00006	-0.00050	-3.13039
D96	-0.00104	0.00000	-0.00032	0.00025	-0.00007	-0.00111
D97	3.13625	0.00001	0.00030	0.00008	0.00038	3.13663
D98	-3.13739	-0.00001	-0.00061	0.00012	-0.00049	-3.13788
D99	-0.00010	0.00000	0.00001	-0.00005	-0.00004	-0.00015
D100	-3.13306	-0.00002	-0.00037	-0.00019	-0.00056	-3.13362
D101	0.00501	0.00002	0.00038	0.00012	0.00050	0.00551
D102	0.00184	0.00001	0.00012	0.00007	0.00019	0.00203
D103	3.13991	0.00004	0.00088	0.00038	0.00125	3.14116
D104	-3.13780	-0.00003	-0.00073	-0.00040	-0.00113	-3.13893
D105	0.00014	-0.00001	-0.00011	-0.00029	-0.00040	-0.00026
D106	0.00026	0.00000	0.00003	-0.00009	-0.00007	0.00020
D107	3.13820	0.00002	0.00064	0.00002	0.00067	3.13886
D108	-0.00431	0.00000	-0.00022	0.00003	-0.00020	-0.00450

```
   D109      -3.13691  -0.00003  -0.00105  -0.00022  -0.00127  -
3.13818
   D110       3.13364   0.00001   0.00039   0.00015   0.00054
3.13418
   D111       0.00104  -0.00001  -0.00043  -0.00011  -0.00054
0.00050
   D112      -0.01561   0.00052   0.01790  -0.00192   0.01598
0.00038
   D113       3.13963   0.00000   0.00421  -0.00620  -0.00198
3.13765
   D114      -0.00497  -0.00060  -0.01763   0.00267  -0.01496  -
0.01993
   D115       3.13405   0.00022   0.00149   0.00085   0.00232
3.13637
         Item               Value     Threshold  Converged?
 Maximum Force            0.001508     0.000450     NO
 RMS     Force            0.000387     0.000300     NO
 Maximum Displacement     0.030808     0.001800     NO
 RMS     Displacement     0.005787     0.001200     NO
 Predicted change in Energy=-7.905895D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.657134   -1.063493   -0.025090
      2          6           0       -0.228333   -1.573719   -0.040743
      3          1           0       -0.161367   -2.662250    0.024175
      4          6           0       -1.758148    0.336044   -0.096244
      5          6           0        0.366741   -1.069357   -1.403135
      6          1           0       -0.177281   -1.545238   -2.224684
      7          6           0        0.529435   -0.873914    1.073600
      8          6           0        0.445652    0.528445    1.028483
      9          6           0       -0.386914    1.034832   -0.157755
     10          6           0        0.309815    0.470292   -1.468818
     11          1           0       -0.238508    0.840282   -2.340143
     12          6           0        1.270255   -1.494717    2.077490
     13          1           0        1.344895   -2.579040    2.109556
     14          6           0        1.094689    1.312553    1.978761
     15          1           0        1.034467    2.396477    1.934064
     16          6           0        1.829542    0.682818    2.991184
     17          1           0        2.336748    1.286151    3.738915
     18          6           0        1.917564   -0.710497    3.040287
     19          1           0        2.493730   -1.190399    3.826698
     20          6           0       -2.808884   -1.844117    0.035030
     21          1           0       -2.732350   -2.927734    0.090121
     22          6           0       -4.064513   -1.222145    0.031164
     23          1           0       -4.965864   -1.826728    0.085446
```

24	6	0	-4.160115	0.169208	-0.039112
25	1	0	-5.135454	0.648004	-0.039377
26	6	0	-3.003688	0.958179	-0.106147
27	1	0	-3.080106	2.040784	-0.157578
28	6	0	1.842562	-1.404035	-1.553467
29	6	0	1.771122	0.894059	-1.610712
30	8	0	2.582232	-0.235338	-1.666890
31	8	0	2.228125	1.996580	-1.686197
32	8	0	2.361282	-2.483810	-1.583324
33	6	0	-0.516270	2.493159	-0.197750
34	7	0	-0.670829	3.643274	-0.210478

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.517250	0.000000			
3	H	2.189925	1.092519	0.000000		
4	C	1.404980	2.447572	3.399114	0.000000	
5	C	2.448492	1.569907	2.203048	2.863262	0.000000
6	H	2.694486	2.184723	2.511042	3.250941	1.094242
7	C	2.454413	1.518453	2.185554	2.839994	2.489756
8	C	2.840069	2.452874	3.399653	2.481686	2.910664
9	C	2.456425	2.615985	3.708421	1.540250	2.558628
10	C	2.881967	2.550879	3.501979	2.485649	1.542100
11	H	3.316071	3.333879	4.226545	2.756564	2.211568
12	C	3.629931	2.595942	2.762025	4.153074	3.621052
13	H	3.983186	2.847718	2.573822	4.795012	3.946508
14	C	4.151330	3.762891	4.604036	3.660313	4.200074
15	H	4.801499	4.610530	5.537907	4.020726	4.857444
16	C	4.929951	4.303416	4.894522	4.745944	4.951762
17	H	5.969895	5.389277	5.969066	5.690283	5.989158
18	C	4.722246	3.852632	4.150690	4.944081	4.719939
19	H	5.664101	4.744855	4.865703	5.983140	5.647112
20	C	1.392665	2.595785	2.771066	2.423712	3.571157
21	H	2.155171	2.849664	2.585495	3.411165	3.909955
22	C	2.413258	3.852928	4.160349	2.786307	4.660105
23	H	3.397417	4.745960	4.876991	3.872988	5.588037
24	C	2.790100	4.300780	4.900117	2.408432	4.887436
25	H	3.876614	5.386641	5.975229	3.392161	5.923117
26	C	2.430418	3.757310	4.604702	1.392307	4.141603
27	H	3.417446	4.605529	5.538105	2.158119	4.806781
28	C	3.834028	2.570162	2.843904	4.256346	1.520742
29	C	4.254309	3.542958	4.365169	3.880817	2.422886
30	O	4.620992	3.512107	4.034469	4.651054	2.381922
31	O	5.217141	4.635595	5.508153	4.601706	3.597895
32	O	4.537957	3.148639	2.996606	5.208904	2.451802
33	C	3.739137	4.080080	5.172373	2.491126	3.863183
34	N	4.812569	5.238476	6.330423	3.483258	4.970702

		6	7	8	9	10
6	H	0.000000				
7	C	3.439302	0.000000			
8	C	3.907851	1.405583	0.000000		

This journal is © The Royal Society of Chemistry 2014

9	C	3.312536	2.449335	1.535173	0.000000	
10	C	2.207024	2.884270	2.501669	1.588402	0.000000
11	H	2.389097	3.896389	3.451516	2.196063	1.093965
12	C	4.539451	1.393559	2.423544	3.760472	4.166534
13	H	4.708651	2.155374	3.410838	4.604338	4.813998
14	C	5.239640	2.432995	1.392516	2.614762	3.634726
15	H	5.856674	3.419198	2.157852	2.872301	3.976797
16	C	6.016382	2.791204	2.406486	3.866835	4.716604
17	H	7.064107	3.877649	3.390693	4.760833	5.647527
18	C	5.727572	2.412771	2.783676	4.310947	4.930633
19	H	6.624155	3.396787	3.870277	5.396816	5.964047
20	C	3.481518	3.628263	4.148253	3.767154	4.164652
21	H	3.714565	3.978021	4.788047	4.611338	4.819921
22	C	4.505975	4.723589	4.939717	4.319071	4.924331
23	H	5.324140	5.664151	5.976677	5.405040	5.960271
24	C	4.855823	4.931339	4.741508	3.873039	4.702657
25	H	5.845456	5.970420	5.683606	4.765741	5.632570
26	C	4.329419	4.151062	3.656502	2.618405	3.615828
27	H	5.055578	4.800005	4.015581	2.874931	3.959465
28	C	2.133128	2.984429	3.514584	3.587010	2.422721
29	C	3.181730	3.445729	2.975886	2.605383	1.528113
30	O	3.105138	3.483108	3.523262	3.564638	2.387681
31	O	4.315139	4.329176	3.564003	3.177974	2.461041
32	O	2.781467	3.606477	4.423217	4.686754	3.598380
33	C	4.531227	3.747934	2.507797	1.464599	2.527849
34	N	5.587600	4.847110	3.533231	2.624378	3.551465

		11	12	13	14	15
11	H	0.000000				
12	C	5.219585	0.000000			
13	H	5.830845	1.087363	0.000000		
14	C	4.544600	2.814486	3.901821	0.000000	
15	H	4.723458	3.900969	4.988280	1.086515	0.000000
16	C	5.720549	2.426787	3.413484	1.400563	2.164780
17	H	6.617075	3.410420	4.310254	2.154425	2.487216
18	C	6.000216	1.400353	2.164640	2.428310	3.414217
19	H	7.044055	2.156207	2.489322	3.411298	4.310126
20	C	4.410700	4.575270	4.700813	5.383357	6.029952
21	H	5.130632	4.692976	4.563292	6.016080	6.777630
22	C	4.951265	5.720271	5.951686	6.069201	6.535676
23	H	5.945109	6.554971	6.669983	7.083080	7.566824
24	C	4.596095	6.061152	6.517267	5.743867	5.986471
25	H	5.413925	7.078523	7.551599	6.582492	6.709662
26	C	3.556805	5.389949	6.027556	4.611845	4.747405
27	H	3.778819	6.034976	6.786996	4.745859	4.629385
28	C	3.160169	3.676902	3.878923	4.518385	5.221090
29	C	2.138591	4.422664	5.107297	3.676550	3.919868
30	O	3.093024	4.162656	4.613620	4.230782	4.721111
31	O	2.801597	5.222261	6.010336	3.896728	3.832888
32	O	4.287338	3.945910	3.831380	5.357712	6.160329
33	C	2.720111	4.926616	5.874930	2.954018	2.637947
34	N	3.546709	5.949921	6.939950	3.652682	3.010249

		16	17	18	19	20

This journal is © The Royal Society of Chemistry 2014

16	C	0.000000				
17	H	1.086448	0.000000			
18	C	1.396956	2.156479	0.000000		
19	H	2.155961	2.483073	1.086607	0.000000	
20	C	6.053036	7.070705	5.714541	6.551473	0.000000
21	H	6.501009	7.534340	5.936440	6.655242	1.087712
22	C	6.865165	7.811217	6.715792	7.577442	1.401239
23	H	7.805042	8.738764	7.573549	8.369433	2.157640
24	C	6.732197	7.598044	6.869844	7.814516	2.425860
25	H	7.595834	8.397412	7.815045	8.748183	3.410151
26	C	5.747120	6.588802	6.074804	7.092619	2.812604
27	H	5.988608	6.715239	6.540076	7.575133	3.899117
28	C	5.000898	5.957401	4.646418	5.423637	4.934870
29	C	4.607113	5.393717	4.922178	5.867926	5.584132
30	O	4.806996	5.621202	4.777559	5.576691	5.877825
31	O	4.874704	5.472508	5.455673	6.373334	6.563919
32	O	5.588954	6.522226	4.971851	5.564063	5.455170
33	C	4.353099	5.009382	5.164479	6.230961	4.911438
34	N	5.026609	5.495385	6.018520	7.048235	5.894321

		21	22	23	24	25
21	H	0.000000				
22	C	2.164986	0.000000			
23	H	2.490144	1.086692	0.000000		
24	C	3.412661	1.396403	2.156039	0.000000	
25	H	4.310171	2.156235	2.483674	1.086523	0.000000
26	C	3.900316	2.428584	3.412118	1.401532	2.155249
27	H	4.986829	3.413413	4.309617	2.164082	2.485612
28	C	5.094395	6.118634	7.015652	6.387526	7.429404
29	C	6.146560	6.420959	7.461006	6.178585	7.087343
30	O	6.211350	6.930830	7.910560	6.947846	7.936736
31	O	7.211830	7.273707	8.337259	6.845567	7.665049
32	O	5.379830	6.744569	7.543448	7.207753	8.270011
33	C	5.863442	5.142559	6.208100	4.324756	4.976599
34	N	6.893358	5.936985	6.961022	4.926827	5.379015

		26	27	28	29	30
26	C	0.000000				
27	H	1.086517	0.000000			
28	C	5.582197	6.168302	0.000000		
29	C	5.006659	5.192398	2.299917	0.000000	
30	O	5.921393	6.286559	1.387743	1.391615	0.000000
31	O	5.562976	5.524124	3.424976	1.195869	2.259917
32	O	6.543106	7.218961	1.198280	3.429145	2.260847
33	C	2.924346	2.603749	4.752913	3.128218	4.382212
34	N	3.558490	2.894026	5.796213	3.934713	5.267559

		31	32	33	34	
31	O	0.000000				
32	O	4.483549	0.000000			
33	C	3.161292	5.913572	0.000000		
34	N	3.645995	6.972773	1.160524	0.000000	

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96

This journal is © The Royal Society of Chemistry 2014

```
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.657308   -1.064523   -0.015900
      2          6           0       -0.228145   -1.573939   -0.010018
      3          1           0       -0.161133   -2.661043    0.075502
      4          6           0       -1.758485    0.333394   -0.113673
      5          6           0        0.378215   -1.094326   -1.376365
      6          1           0       -0.158538   -1.585637   -2.193601
      7          6           0        0.519733   -0.853199    1.097643
      8          6           0        0.435564    0.548031    1.025996
      9          6           0       -0.387163    1.031902   -0.176396
     10          6           0        0.321001    0.443812   -1.470874
     11          1           0       -0.220096    0.797309   -2.353491
     12          6           0        1.252331   -1.454889    2.119051
     13          1           0        1.327294   -2.538385    2.171714
     14          6           0        1.076063    1.349962    1.967149
     15          1           0        1.015626    2.432837    1.901987
     16          6           0        1.802627    0.739495    2.997203
     17          1           0        2.303124    1.356852    3.737975
     18          6           0        1.890997   -0.652617    3.072704
     19          1           0        2.460718   -1.117550    3.872684
     20          6           0       -2.809097   -1.844723    0.048803
     21          1           0       -2.732438   -2.927087    0.124491
     22          6           0       -4.064991   -1.223817    0.022820
     23          1           0       -4.966438   -1.827936    0.080571
     24          6           0       -4.160759    0.165938   -0.073878
     25          1           0       -5.136325    0.643957   -0.091244
     26          6           0       -3.004239    0.954360   -0.145609
     27          1           0       -3.080814    2.035780   -0.217617
     28          6           0        1.855445   -1.430670   -1.507970
     29          6           0        1.783228    0.865929   -1.608134
     30          8           0        2.595409   -0.263735   -1.636611
     31          8           0        2.240248    1.967197   -1.700027
     32          8           0        2.374996   -2.510444   -1.513529
     33          6           0       -0.516979    2.489153   -0.244339
     34          7           0       -0.672059    3.638730   -0.279558
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3754929      0.2678991
0.2564833
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
```

```
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1879.0357409524 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A)
 Harris functional with IExCor=  402 diagonalized for initial guess.
```

This journal is © The Royal Society of Chemistry 2014

```
 ExpMin= 4.38D-02 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=2 IRadAn=
0 AccDes= 0.00D+00
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=
0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1011.11154465     A.U. after   14 cycles
             Convg  =    0.4274D-08             -V/T =  2.0093
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000119046    0.000050960    0.000020704
      2        6           0.000024084    0.000063212   -0.000012466
      3        1          -0.000008609    0.000006121   -0.000006965
      4        6          -0.000077640   -0.000062108    0.000018503
      5        6           0.000088776   -0.000117778    0.000126955
      6        1           0.000027865    0.000001565    0.000002243
      7        6           0.000020400    0.000022296    0.000039270
      8        6           0.000003804    0.000018177    0.000024941
      9        6           0.000030944   -0.000060474   -0.000056949
     10        6           0.000036135    0.000091316   -0.000026811
     11        1          -0.000016891   -0.000025546   -0.000008149
     12        6          -0.000009496    0.000051041    0.000021642
     13        1          -0.000002841    0.000020197    0.000002373
     14        6          -0.000024931   -0.000039955    0.000002107
     15        1           0.000010532   -0.000019567    0.000000268
     16        6          -0.000020342   -0.000045250   -0.000032941
     17        1          -0.000013016   -0.000004864   -0.000004340
     18        6          -0.000017707    0.000032314   -0.000046857
     19        1          -0.000017956    0.000009939    0.000001950
     20        6           0.000009382    0.000036693   -0.000006498
     21        1          -0.000004206    0.000021012   -0.000006686
     22        6           0.000044132    0.000048627   -0.000016040
     23        1           0.000011318    0.000008680   -0.000003010
     24        6           0.000052317   -0.000053579   -0.000007725
     25        1           0.000015077    0.000003139   -0.000009406
```

This journal is © The Royal Society of Chemistry 2014

```
     26        6           0.000060219   -0.000045073    0.000000353
     27        1          -0.000000394   -0.000006764   -0.000003992
     28        6          -0.000036888    0.000182789   -0.000449079
     29        6          -0.000071024    0.000146137    0.000273240
     30        8           0.000035838   -0.000173945    0.000084973
     31        8          -0.000052840   -0.000124478   -0.000092899
     32        8          -0.000012788   -0.000024915    0.000169272
     33        6           0.000062612    0.000040730    0.000014850
     34        7          -0.000026819   -0.000050648   -0.000012831
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000449079 RMS     0.000074623


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000127744 RMS     0.000031401
 Search for a local minimum.
 Step number   4 out of a maximum of  204
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
 DE= -7.05D-05 DEPred=-7.91D-05 R= 8.92D-01
 SS=  1.41D+00  RLast= 5.16D-02 DXNew= 5.0454D-01 1.5478D-01
 Trust test= 8.92D-01 RLast= 5.16D-02 DXMaxT set to 3.00D-01
     Eigenvalues ---    0.00438   0.00840   0.01061   0.01149
0.01166
     Eigenvalues ---    0.01424   0.01483   0.01579   0.01819
0.02114
     Eigenvalues ---    0.02119   0.02128   0.02129   0.02130
0.02130
     Eigenvalues ---    0.02151   0.02153   0.02159   0.02161
0.02163
     Eigenvalues ---    0.02169   0.02791   0.03301   0.03883
0.04249
     Eigenvalues ---    0.04794   0.04853   0.04973   0.05289
0.05397
     Eigenvalues ---    0.05558   0.06484   0.06650   0.07567
0.08567
     Eigenvalues ---    0.08761   0.09769   0.10129   0.12274
0.15875
     Eigenvalues ---    0.15999   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16003   0.16374   0.20391
0.21820
     Eigenvalues ---    0.22000   0.22006   0.22291   0.22617
0.22652
     Eigenvalues ---    0.24482   0.24588   0.24710   0.24810
0.24993
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.26383   0.27350   0.27723   0.28792
0.29016
     Eigenvalues ---    0.29750   0.29880   0.34373   0.34410
0.34553
     Eigenvalues ---    0.35141   0.35183   0.35240   0.35252
0.35259
     Eigenvalues ---    0.35267   0.35274   0.35325   0.36501
0.37029
     Eigenvalues ---    0.40120   0.42094   0.42134   0.43447
0.44150
     Eigenvalues ---    0.44827   0.45870   0.46010   0.46126
0.46481
     Eigenvalues ---    0.46521   0.46936   0.48130   1.04612
1.07262
     Eigenvalues ---
1.275881000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     4    3    2    1
 RFO step:  Lambda=-8.09985449D-07.
 DIIS coeffs:      0.46768      0.19493      0.15933      0.17807
 Iteration  1 RMS(Cart)=  0.00065791 RMS(Int)=  0.00000617
 Iteration  2 RMS(Cart)=  0.00000087 RMS(Int)=  0.00000613
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                   (DIIS)     (GDIIS)  (Total)
    R1        2.86719   0.00002  -0.00025   0.00029   0.00004
2.86723
    R2        2.65503  -0.00009   0.00007  -0.00023  -0.00016
2.65487
    R3        2.63176  -0.00008  -0.00002  -0.00013  -0.00016
2.63160
    R4        2.06456  -0.00001   0.00000  -0.00002  -0.00002
2.06454
    R5        2.96669  -0.00001   0.00033  -0.00045  -0.00012
2.96657
    R6        2.86946   0.00000   0.00033  -0.00035  -0.00002
2.86944
    R7        2.91065  -0.00001  -0.00024   0.00020  -0.00004
2.91062
    R8        2.63108  -0.00012  -0.00001  -0.00019  -0.00020
2.63088
    R9        2.06782  -0.00001  -0.00007   0.00004  -0.00003
2.06778
   R10        2.91415  -0.00001  -0.00043   0.00041  -0.00002
2.91412
   R11        2.87379  -0.00008   0.00046  -0.00064  -0.00018
2.87361
   R12        2.65617  -0.00006   0.00007  -0.00018  -0.00011
2.65606
   R13        2.63344  -0.00005  -0.00004  -0.00009  -0.00012
2.63332
   R14        2.90106  -0.00005   0.00017  -0.00033  -0.00016
2.90089
   R15        2.63147  -0.00007   0.00001  -0.00015  -0.00014
2.63133
```

R16	3.00165	-0.00008	0.00049	-0.00079	-0.00030
3.00135					
R17	2.76769	-0.00001	0.00003	-0.00008	-0.00005
2.76764					
R18	2.06729	0.00001	-0.00008	0.00008	0.00000
2.06730					
R19	2.88772	-0.00009	0.00034	-0.00053	-0.00020
2.88752					
R20	2.05482	-0.00002	-0.00003	-0.00002	-0.00005
2.05477					
R21	2.64628	-0.00007	-0.00005	-0.00010	-0.00015
2.64614					
R22	2.05322	-0.00002	-0.00004	-0.00001	-0.00005
2.05317					
R23	2.64668	-0.00006	-0.00006	-0.00007	-0.00013
2.64655					
R24	2.05309	-0.00001	0.00001	-0.00005	-0.00004
2.05305					
R25	2.63986	-0.00008	-0.00011	-0.00005	-0.00015
2.63971					
R26	2.05339	-0.00001	0.00001	-0.00004	-0.00004
2.05335					
R27	2.05548	-0.00002	-0.00001	-0.00005	-0.00005
2.05543					
R28	2.64796	-0.00007	-0.00009	-0.00007	-0.00015
2.64781					
R29	2.05355	-0.00001	0.00001	-0.00005	-0.00004
2.05351					
R30	2.63882	-0.00008	-0.00008	-0.00007	-0.00015
2.63867					
R31	2.05323	-0.00001	0.00002	-0.00006	-0.00004
2.05320					
R32	2.64851	-0.00006	-0.00009	-0.00005	-0.00014
2.64837					
R33	2.05322	-0.00001	0.00000	-0.00003	-0.00003
2.05319					
R34	2.62245	-0.00011	0.00009	-0.00025	-0.00015
2.62231					
R35	2.26442	0.00001	-0.00035	0.00032	-0.00003
2.26439					
R36	2.62977	0.00009	-0.00034	0.00043	0.00009
2.62986					
R37	2.25987	-0.00013	-0.00015	0.00006	-0.00009
2.25978					
R38	2.19307	-0.00005	-0.00004	0.00001	-0.00003
2.19305					
A1	1.98468	-0.00002	-0.00016	0.00008	-0.00007
1.98460					
A2	2.20278	0.00001	0.00024	-0.00020	0.00004
2.20282					
A3	2.09564	0.00001	-0.00008	0.00011	0.00003
2.09567					

This journal is © The Royal Society of Chemistry 2014

A4	1.97378	0.00000	-0.00002	0.00001	-0.00001
1.97377					
A5	1.83161	0.00002	0.00014	-0.00022	-0.00009
1.83152					
A6	1.88325	-0.00001	-0.00003	0.00007	0.00003
1.88328					
A7	1.92669	-0.00001	-0.00006	-0.00004	-0.00010
1.92659					
A8	1.96599	0.00001	-0.00003	0.00008	0.00006
1.96605					
A9	1.87511	0.00001	0.00001	0.00009	0.00011
1.87522					
A10	1.97136	0.00002	0.00017	-0.00015	0.00002
1.97138					
A11	2.10573	0.00001	0.00000	0.00003	0.00003
2.10576					
A12	2.20609	-0.00003	-0.00017	0.00013	-0.00005
2.20604					
A13	1.90010	0.00001	0.00049	-0.00053	-0.00004
1.90006					
A14	1.92168	-0.00004	0.00006	-0.00017	-0.00011
1.92157					
A15	1.96377	0.00004	-0.00057	0.00086	0.00029
1.96406					
A16	1.96478	0.00001	-0.00016	0.00018	0.00003
1.96481					
A17	1.88868	-0.00003	0.00003	-0.00017	-0.00015
1.88853					
A18	1.82486	0.00000	0.00009	-0.00012	-0.00002
1.82484					
A19	1.98943	0.00000	-0.00006	0.00005	0.00000
1.98942					
A20	2.20018	0.00001	0.00017	-0.00016	0.00002
2.20019					
A21	2.09355	0.00000	-0.00012	0.00011	-0.00001
2.09354					
A22	1.96734	0.00000	-0.00008	0.00003	-0.00004
1.96729					
A23	2.10843	0.00000	0.00001	0.00000	0.00002
2.10845					
A24	2.20725	0.00000	0.00005	-0.00003	0.00002
2.20727					
A25	1.87791	0.00000	-0.00022	0.00024	0.00003
1.87794					
A26	1.83612	0.00001	0.00029	0.00001	0.00029
1.83641					
A27	1.95433	0.00000	-0.00020	0.00029	0.00009
1.95442					
A28	1.85737	0.00001	-0.00006	-0.00016	-0.00022
1.85715					
A29	1.97953	-0.00001	0.00002	-0.00009	-0.00006
1.97946					

This journal is © The Royal Society of Chemistry 2014

A30	1.94991	0.00000	0.00018	-0.00029	-0.00011
1.94980					
A31	1.91334	0.00002	-0.00005	0.00008	0.00003
1.91337					
A32	1.97154	-0.00002	-0.00005	0.00004	0.00000
1.97153					
A33	1.81886	-0.00001	-0.00009	0.00006	-0.00004
1.81882					
A34	1.89374	0.00000	0.00019	-0.00002	0.00017
1.89390					
A35	1.97963	-0.00003	-0.00052	-0.00005	-0.00057
1.97906					
A36	1.88763	0.00003	0.00050	-0.00011	0.00039
1.88803					
A37	2.09667	0.00000	-0.00013	0.00013	0.00000
2.09667					
A38	2.08466	0.00000	0.00008	-0.00009	-0.00001
2.08465					
A39	2.10185	0.00000	0.00005	-0.00005	0.00001
2.10186					
A40	2.10347	0.00001	-0.00027	0.00029	0.00002
2.10349					
A41	2.07678	0.00000	0.00004	-0.00007	-0.00003
2.07675					
A42	2.10293	-0.00001	0.00023	-0.00022	0.00001
2.10294					
A43	2.08605	0.00000	0.00005	-0.00007	-0.00001
2.08604					
A44	2.10241	0.00001	-0.00004	0.00006	0.00002
2.10243					
A45	2.09471	0.00000	-0.00001	0.00000	-0.00001
2.09470					
A46	2.10048	0.00000	0.00003	-0.00002	0.00001
2.10049					
A47	2.08905	0.00000	-0.00002	0.00002	0.00000
2.08905					
A48	2.09365	0.00000	-0.00001	0.00000	-0.00001
2.09363					
A49	2.09718	0.00001	-0.00009	0.00012	0.00002
2.09721					
A50	2.08536	-0.00002	0.00003	-0.00008	-0.00005
2.08531					
A51	2.10063	0.00001	0.00006	-0.00003	0.00003
2.10066					
A52	2.08997	0.00000	0.00000	-0.00002	-0.00001
2.08996					
A53	2.09874	0.00000	0.00005	-0.00004	0.00001
2.09874					
A54	2.09447	0.00000	-0.00005	0.00006	0.00000
2.09448					
A55	2.09502	0.00000	-0.00007	0.00009	0.00001
2.09504					

A56	2.10228	0.00001	-0.00003	0.00007	0.00003	2.10232
A57	2.08587	-0.00001	0.00010	-0.00015	-0.00005	2.08583
A58	2.07860	-0.00001	0.00003	-0.00008	-0.00005	2.07855
A59	2.10422	0.00001	-0.00036	0.00038	0.00002	2.10424
A60	2.10034	0.00000	0.00033	-0.00030	0.00003	2.10037
A61	1.91771	0.00004	-0.00018	0.00022	0.00006	1.91777
A62	2.24065	-0.00007	-0.00011	-0.00006	-0.00016	2.24049
A63	2.12481	0.00002	0.00023	-0.00014	0.00011	2.12492
A64	1.91353	0.00000	0.00009	-0.00010	0.00002	1.91355
A65	2.24846	0.00000	-0.00041	0.00027	-0.00009	2.24837
A66	2.12109	0.00000	0.00015	-0.00020	0.00000	2.12109
A67	1.94928	-0.00004	-0.00001	-0.00008	-0.00009	1.94919
A68	3.09583	-0.00008	-0.00134	0.00069	-0.00065	3.09519
A69	3.11724	0.00001	-0.00077	0.00093	0.00015	3.11739
D1	3.13243	0.00000	-0.00001	0.00024	0.00023	3.13266
D2	-1.04964	-0.00001	0.00000	0.00005	0.00005	-1.04960
D3	0.94594	0.00000	0.00007	0.00007	0.00014	0.94608
D4	-0.02308	0.00000	-0.00027	0.00015	-0.00012	-0.02320
D5	2.07803	-0.00001	-0.00026	-0.00004	-0.00030	2.07773
D6	-2.20957	0.00000	-0.00019	-0.00002	-0.00021	-2.20978
D7	-0.01161	0.00000	0.00010	-0.00037	-0.00027	-0.01188
D8	3.12980	0.00000	0.00005	-0.00025	-0.00020	3.12960
D9	-3.14023	0.00000	0.00034	-0.00028	0.00006	-3.14017
D10	0.00119	0.00000	0.00030	-0.00017	0.00013	0.00131
D11	0.01469	0.00000	0.00023	-0.00005	0.00018	0.01488
D12	-3.13283	0.00000	0.00011	0.00017	0.00028	-3.13255

This journal is © The Royal Society of Chemistry 2014

D13	3.14156	0.00000	-0.00005	-0.00014	-0.00019	3.14138
D14	-0.00596	0.00000	-0.00017	0.00008	-0.00009	-0.00605
D15	-1.12091	0.00000	0.00009	0.00074	0.00083	-1.12008
D16	1.04075	0.00000	0.00027	0.00050	0.00077	1.04152
D17	3.06878	0.00000	0.00008	0.00077	0.00085	3.06963
D18	1.01113	0.00000	0.00012	0.00059	0.00071	1.01184
D19	-3.11039	-0.00001	0.00030	0.00035	0.00065	-3.10974
D20	-1.08237	0.00000	0.00011	0.00062	0.00073	-1.08163
D21	-3.12218	0.00000	0.00007	0.00072	0.00079	-3.12139
D22	-0.96052	0.00000	0.00024	0.00049	0.00073	-0.95979
D23	1.06751	0.00000	0.00006	0.00075	0.00081	1.06832
D24	-0.93500	-0.00001	-0.00005	0.00025	0.00020	-0.93480
D25	2.21510	-0.00001	0.00064	-0.00054	0.00010	2.21519
D26	-3.12611	0.00000	0.00002	0.00012	0.00015	-3.12596
D27	0.02399	0.00000	0.00070	-0.00066	0.00004	0.02403
D28	1.03154	0.00001	0.00010	0.00006	0.00016	1.03170
D29	-2.10155	0.00001	0.00078	-0.00072	0.00006	-2.10148
D30	-0.93024	-0.00002	-0.00029	0.00038	0.00008	-0.93015
D31	1.04497	0.00000	-0.00032	0.00030	-0.00002	1.04495
D32	-3.11681	0.00000	-0.00003	0.00012	0.00009	-3.11672
D33	2.21155	-0.00001	-0.00024	0.00025	0.00001	2.21156
D34	-2.09643	0.00000	-0.00027	0.00018	-0.00009	-2.09652
D35	0.02498	0.00000	0.00002	-0.00001	0.00002	0.02499
D36	0.00405	0.00000	-0.00020	0.00011	-0.00009	0.00396
D37	3.13771	0.00000	-0.00030	0.00025	-0.00005	3.13765
D38	-3.13775	0.00000	-0.00025	0.00024	-0.00002	-3.13777

This journal is © The Royal Society of Chemistry 2014

D39	-0.00409	0.00000	-0.00036	0.00038	0.00002	-0.00407
D40	-0.03931	0.00001	-0.00042	-0.00067	-0.00109	-0.04040
D41	-2.15346	0.00001	-0.00059	-0.00073	-0.00132	-2.15478
D42	2.08503	-0.00002	-0.00112	-0.00065	-0.00177	2.08326
D43	2.08432	0.00001	0.00015	-0.00134	-0.00119	2.08313
D44	-0.02982	0.00000	-0.00002	-0.00140	-0.00142	-0.03125
D45	-2.07452	-0.00002	-0.00054	-0.00133	-0.00187	-2.07639
D46	-2.15270	-0.00002	0.00016	-0.00153	-0.00137	-2.15407
D47	2.01634	-0.00002	-0.00001	-0.00158	-0.00160	2.01474
D48	-0.02836	-0.00005	-0.00053	-0.00151	-0.00204	-0.03040
D49	-2.06664	0.00009	-0.00024	0.00254	0.00231	-2.06433
D50	1.07964	-0.00005	-0.00266	-0.00154	-0.00419	1.07545
D51	2.11645	0.00006	-0.00052	0.00278	0.00226	2.11872
D52	-1.02045	-0.00008	-0.00294	-0.00129	-0.00423	-1.02468
D53	0.01863	0.00006	-0.00040	0.00272	0.00232	0.02095
D54	-3.11827	-0.00008	-0.00282	-0.00136	-0.00418	-3.12245
D55	-0.01186	0.00000	-0.00019	-0.00017	-0.00036	-0.01222
D56	-3.13490	0.00000	0.00045	-0.00050	-0.00005	-3.13495
D57	3.12180	0.00000	-0.00082	0.00056	-0.00026	3.12154
D58	-0.00125	0.00000	-0.00018	0.00023	0.00004	-0.00120
D59	0.00130	0.00000	-0.00077	0.00084	0.00007	0.00137
D60	3.14096	0.00000	-0.00088	0.00093	0.00005	3.14101
D61	-3.13133	0.00000	-0.00005	0.00002	-0.00003	-3.13136
D62	0.00834	0.00000	-0.00016	0.00011	-0.00005	0.00829
D63	0.94134	0.00001	0.00023	0.00003	0.00025	0.94159
D64	-1.01952	0.00000	0.00002	-0.00002	0.00001	-1.01951

This journal is © The Royal Society of Chemistry 2014

D65	3.11277	0.00000	-0.00018	0.00052	0.00034	3.11312
D66	-2.22007	0.00001	-0.00046	0.00038	-0.00007	-2.22014
D67	2.10226	0.00000	-0.00066	0.00034	-0.00032	2.10194
D68	-0.04863	0.00000	-0.00086	0.00087	0.00001	-0.04861
D69	3.13156	0.00000	0.00015	-0.00030	-0.00015	3.13140
D70	-0.00700	0.00000	0.00037	-0.00039	-0.00003	-0.00703
D71	0.01124	0.00000	0.00088	-0.00069	0.00020	0.01144
D72	-3.12732	0.00000	0.00110	-0.00078	0.00032	-3.12699
D73	-0.97526	0.00000	0.00055	0.00026	0.00080	-0.97445
D74	1.18520	-0.00001	0.00058	0.00035	0.00093	1.18612
D75	-3.00007	0.00002	0.00101	0.00016	0.00118	-2.99890
D76	1.01434	0.00000	0.00041	0.00046	0.00087	1.01521
D77	-3.10840	-0.00001	0.00044	0.00056	0.00099	-3.10740
D78	-1.01048	0.00002	0.00087	0.00037	0.00124	-1.00924
D79	-3.09955	0.00000	0.00051	0.00007	0.00057	-3.09897
D80	-0.93909	-0.00001	0.00054	0.00016	0.00070	-0.93839
D81	1.15882	0.00001	0.00097	-0.00003	0.00095	1.15977
D82	0.03028	0.00003	0.00133	-0.00011	0.00121	0.03149
D83	-3.12740	-0.00004	0.00026	-0.00295	-0.00269	-3.13009
D84	2.11012	0.00003	0.00093	0.00000	0.00093	2.11105
D85	-1.04756	-0.00004	-0.00014	-0.00284	-0.00298	-1.05054
D86	-2.07169	0.00004	0.00119	-0.00014	0.00105	-2.07064
D87	1.05381	-0.00003	0.00012	-0.00298	-0.00286	1.05096
D88	-0.00719	0.00000	0.00032	-0.00027	0.00005	-0.00714
D89	3.13825	0.00000	0.00021	-0.00031	-0.00009	3.13816
D90	3.13247	0.00000	0.00021	-0.00018	0.00003	3.13250

```
   D91       -0.00528  -0.00001   0.00010  -0.00022  -0.00011  -
0.00539
   D92       -3.13823   0.00000  -0.00026   0.00031   0.00004  -
3.13819
   D93        0.00816   0.00000  -0.00020   0.00023   0.00003
0.00819
   D94        0.00640   0.00001  -0.00004   0.00022   0.00017
0.00657
   D95       -3.13039   0.00000   0.00001   0.00014   0.00015  -
3.13024
   D96       -0.00111   0.00000  -0.00014   0.00010  -0.00004  -
0.00115
   D97        3.13663   0.00000  -0.00003   0.00014   0.00011
3.13673
   D98       -3.13788   0.00000  -0.00008   0.00003  -0.00006  -
3.13794
   D99       -0.00015   0.00000   0.00003   0.00006   0.00009  -
0.00006
   D100      -3.13362   0.00000   0.00009  -0.00006   0.00002  -
3.13360
   D101       0.00551   0.00000  -0.00005   0.00007   0.00002
0.00553
   D102       0.00203   0.00000  -0.00003   0.00015   0.00012
0.00215
   D103       3.14116   0.00000  -0.00017   0.00029   0.00012
3.14128
   D104      -3.13893   0.00000   0.00019  -0.00019  -0.00001  -
3.13893
   D105      -0.00026   0.00000   0.00015  -0.00014   0.00001  -
0.00025
   D106       0.00020   0.00000   0.00005  -0.00005  -0.00001
0.00019
   D107       3.13886   0.00000   0.00001   0.00000   0.00001
3.13887
   D108      -0.00450   0.00000  -0.00002   0.00005   0.00002  -
0.00448
   D109      -3.13818   0.00000   0.00008  -0.00010  -0.00001  -
3.13820
   D110       3.13418   0.00000  -0.00006   0.00010   0.00004
3.13422
   D111       0.00050   0.00000   0.00004  -0.00004   0.00000
0.00050
   D112       0.00038  -0.00005   0.00131  -0.00296  -0.00165  -
0.00127
   D113       3.13765   0.00008   0.00353   0.00080   0.00434  -
3.14120
   D114      -0.01993   0.00001  -0.00167   0.00191   0.00024  -
0.01969
   D115       3.13637   0.00007  -0.00069   0.00450   0.00381
3.14018
         Item               Value     Threshold  Converged?
 Maximum Force            0.000128     0.000450     YES
```

This journal is © The Royal Society of Chemistry 2014

```
 RMS     Force            0.000031     0.000300     YES
 Maximum Displacement     0.004459     0.001800     NO
 RMS     Displacement     0.000658     0.001200     YES
 Predicted change in Energy=-2.272044D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.657204   -1.063478   -0.024977
      2          6           0       -0.228331   -1.573564   -0.040869
      3          1           0       -0.161255   -2.662085    0.023915
      4          6           0       -1.758270    0.335963   -0.096253
      5          6           0        0.366290   -1.069180   -1.403375
      6          1           0       -0.178453   -1.544525   -2.224732
      7          6           0        0.529574   -0.873743    1.073357
      8          6           0        0.445460    0.528545    1.028450
      9          6           0       -0.387092    1.034820   -0.157735
     10          6           0        0.310069    0.470507   -1.468476
     11          1           0       -0.237398    0.841079   -2.340094
     12          6           0        1.270686   -1.494469    2.076988
     13          1           0        1.345565   -2.578754    2.108918
     14          6           0        1.094479    1.312653    1.978630
     15          1           0        1.034116    2.396545    1.934012
     16          6           0        1.829632    0.682969    2.990770
     17          1           0        2.336817    1.286309    3.738481
     18          6           0        1.917991   -0.710251    3.039676
     19          1           0        2.494332   -1.190100    3.825964
     20          6           0       -2.808833   -1.844140    0.035059
     21          1           0       -2.732254   -2.927730    0.090071
     22          6           0       -4.064405   -1.222233    0.031098
     23          1           0       -4.965721   -1.826835    0.085338
     24          6           0       -4.160039    0.169037   -0.039216
     25          1           0       -5.135369    0.647809   -0.039562
     26          6           0       -3.003721    0.958038   -0.106210
     27          1           0       -3.080168    2.040622   -0.157688
     28          6           0        1.841742   -1.404475   -1.554983
     29          6           0        1.771638    0.893660   -1.608353
     30          8           0        2.582227   -0.236115   -1.665577
     31          8           0        2.228892    1.995927   -1.685287
     32          8           0        2.360178   -2.484450   -1.581705
     33          6           0       -0.516401    2.493125   -0.197746
     34          7           0       -0.671671    3.643130   -0.210558
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  C    1.517273   0.000000
```

This journal is © The Royal Society of Chemistry 2014

3	H	2.189931	1.092507	0.000000		
4	C	1.404895	2.447463	3.398998	0.000000	
5	C	2.448375	1.569841	2.202908	2.862996	0.000000
6	H	2.693888	2.184626	2.511105	3.249997	1.094224
7	C	2.454452	1.518443	2.185575	2.840001	2.489790
8	C	2.839972	2.452815	3.399604	2.481627	2.910801
9	C	2.456352	2.615823	3.708248	1.540231	2.558518
10	C	2.882180	2.550718	3.501786	2.485785	1.542088
11	H	3.317070	3.334220	4.226877	2.757357	2.211554
12	C	3.629952	2.595886	2.762045	4.153075	3.621012
13	H	3.983239	2.847655	2.573847	4.795013	3.946390
14	C	4.151168	3.762772	4.603946	3.660224	4.200160
15	H	4.801313	4.610390	5.537790	4.020621	4.857509
16	C	4.929791	4.303253	4.894409	4.745858	4.951758
17	H	5.969700	5.389095	5.968934	5.690174	5.989155
18	C	4.722170	3.852501	4.150630	4.944038	4.719884
19	H	5.664012	4.744716	4.865640	5.983083	5.647049
20	C	1.392583	2.595759	2.771070	2.423587	3.570863
21	H	2.155088	2.849656	2.585533	3.411019	3.909675
22	C	2.413082	3.852801	4.160265	2.786117	4.659634
23	H	3.397230	4.745834	4.876916	3.872778	5.587544
24	C	2.789889	4.300580	4.899950	2.408238	4.886897
25	H	3.876384	5.386420	5.975051	3.391940	5.922524
26	C	2.430274	3.757135	4.604545	1.392201	4.141162
27	H	3.417291	4.605319	5.537914	2.158020	4.806316
28	C	3.834034	2.570279	2.843677	4.256419	1.520646
29	C	4.253754	3.541762	4.363908	3.880429	2.422759
30	O	4.620484	3.511080	4.033163	4.650803	2.381832
31	O	5.217119	4.635011	5.507381	4.601954	3.597728
32	O	4.536730	3.147105	2.994527	5.207966	2.451607
33	C	3.739078	4.079897	5.172180	2.491162	3.862991
34	N	4.812263	5.238248	6.330184	3.482975	4.970517

		6	7	8	9	10
6	H	0.000000				
7	C	3.439279	0.000000			
8	C	3.907695	1.405526	0.000000		
9	C	3.311952	2.449178	1.535087	0.000000	
10	C	2.207018	2.883766	2.501268	1.588246	0.000000
11	H	2.389119	3.896217	3.451241	2.196050	1.093966
12	C	4.539527	1.393494	2.423431	3.760255	4.165842
13	H	4.708799	2.155294	3.410705	4.604099	4.813314
14	C	5.239473	2.432892	1.392441	2.614631	3.634151
15	H	5.856408	3.419075	2.157773	2.872200	3.976279
16	C	6.016278	2.791053	2.406342	3.866620	4.715834
17	H	7.064001	3.877478	3.390532	4.760611	5.646737
18	C	5.727572	2.412642	2.783522	4.310698	4.929811
19	H	6.624222	3.396646	3.870103	5.396548	5.963197
20	C	3.480708	3.628318	4.148118	3.767016	4.164824
21	H	3.713956	3.978094	4.787928	4.611181	4.820042
22	C	4.504805	4.723599	4.939515	4.318863	4.924440
23	H	5.322975	5.664171	5.976466	5.404813	5.960375
24	C	4.854462	4.931296	4.741284	3.872823	4.702715

This journal is © The Royal Society of Chemistry 2014

25	H	5.843998	5.970368	5.683355	4.765489	5.632586
26	C	4.328175	4.151020	3.656332	2.618262	3.615890
27	H	5.054295	4.799920	4.015389	2.874769	3.959436
28	C	2.132924	2.985235	3.515721	3.587500	2.422614
29	C	3.182377	3.443545	2.974019	2.604675	1.528008
30	O	3.105792	3.481625	3.522536	3.564507	2.387649
31	O	4.315219	4.328141	3.563456	3.178131	2.460853
32	O	2.782371	3.604836	4.422352	4.686196	3.598268
33	C	4.530508	3.747742	2.507650	1.464574	2.527606
34	N	5.586763	4.847016	3.533237	2.624321	3.551297

		11	12	13	14	15
11	H	0.000000				
12	C	5.219168	0.000000			
13	H	5.830501	1.087336	0.000000		
14	C	4.543969	2.814366	3.901675	0.000000	
15	H	4.722733	3.900821	4.988106	1.086489	0.000000
16	C	5.719766	2.426655	3.413329	1.400493	2.164701
17	H	6.616184	3.410267	4.310077	2.154338	2.487120
18	C	5.999521	1.400275	2.164552	2.428195	3.414076
19	H	7.043316	2.156123	2.489231	3.411159	4.309958
20	C	4.411806	4.575393	4.701018	5.383182	6.029734
21	H	5.131659	4.693144	4.563566	6.015927	6.777430
22	C	4.952352	5.720399	5.951912	6.068987	6.535407
23	H	5.946219	6.555143	6.670277	7.082864	7.566543
24	C	4.597041	6.061217	6.517401	5.743650	5.986206
25	H	5.414787	7.078607	7.551767	6.582258	6.709368
26	C	3.557592	5.389962	6.027601	4.611675	4.747202
27	H	3.779304	6.034946	6.786992	4.745679	4.629170
28	C	3.159388	3.677692	3.879342	4.519691	5.222365
29	C	2.138793	4.419938	5.104635	3.674309	3.918029
30	O	3.092831	4.160576	4.611301	4.229931	4.720655
31	O	2.800899	5.220704	6.008658	3.895902	3.832403
32	O	4.287388	3.943741	3.828712	5.356862	6.159775
33	C	2.719698	4.926358	5.874655	2.953822	2.637768
34	N	3.546126	5.949836	6.939817	3.652801	3.010459

		16	17	18	19	20
16	C	0.000000				
17	H	1.086429	0.000000			
18	C	1.396875	2.156385	0.000000		
19	H	2.155867	2.482955	1.086588	0.000000	
20	C	6.052922	7.070555	5.714568	6.551510	0.000000
21	H	6.500923	7.534221	5.936510	6.655332	1.087684
22	C	6.865065	7.811089	6.715856	7.577537	1.401158
23	H	7.804965	8.738660	7.573662	8.369594	2.157543
24	C	6.732095	7.597923	6.869874	7.814571	2.425728
25	H	7.595748	8.397312	7.815109	8.748288	3.410007
26	C	5.747021	6.588683	6.074786	7.092607	2.812497
27	H	5.988501	6.715121	6.540033	7.575097	3.898994
28	C	5.002143	5.958706	4.647435	5.424612	4.934510
29	C	4.604312	5.390940	4.919159	5.864822	5.583643
30	O	4.805484	5.619772	4.775502	5.574480	5.877196
31	O	4.873272	5.471057	5.453929	6.371430	6.563870

This journal is © The Royal Society of Chemistry 2014

32	O	5.587625	6.521008	4.969958	5.562034	5.453677
33	C	4.352835	5.009106	5.164183	6.230642	4.911345
34	N	5.026687	5.495500	6.018496	7.048206	5.893888

		21	22	23	24	25
21	H	0.000000				
22	C	2.164907	0.000000			
23	H	2.490053	1.086672	0.000000		
24	C	3.412514	1.396325	2.155956	0.000000	
25	H	4.310017	2.156158	2.483596	1.086504	0.000000
26	C	3.900181	2.428474	3.411987	1.401457	2.155135
27	H	4.986677	3.413296	4.309478	2.164021	2.485505
28	C	5.093913	6.118123	7.015026	6.387085	7.428892
29	C	6.145951	6.420607	7.460676	6.178354	7.087192
30	O	6.210539	6.930285	7.909969	6.947471	7.936406
31	O	7.211606	7.273797	8.337331	6.845839	7.665388
32	O	5.378122	6.743114	7.541902	7.206490	8.268765
33	C	5.863319	5.142430	6.207950	4.324651	4.976452
34	N	6.892937	5.936396	6.960383	4.926194	5.378269

		26	27	28	29	30
26	C	0.000000				
27	H	1.086501	0.000000			
28	C	5.582017	6.168170	0.000000		
29	C	5.006459	5.192299	2.299823	0.000000	
30	O	5.921185	6.286491	1.387665	1.391661	0.000000
31	O	5.563357	5.524643	3.424850	1.195823	2.259921
32	O	6.542111	7.218134	1.198264	3.429098	2.260830
33	C	2.924317	2.603702	4.753337	3.127815	4.382325
34	N	3.557958	2.893386	5.796813	3.934867	5.268156

		31	32	33	34	
31	O	0.000000				
32	O	4.483497	0.000000			
33	C	3.161744	5.913231	0.000000		
34	N	3.647105	6.972760	1.160510	0.000000	

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.657283	-1.064512	-0.013931
2	6	0	-0.228021	-1.573720	-0.007977
3	1	0	-0.160824	-2.660690	0.078936
4	6	0	-1.758603	0.333162	-0.113782
5	6	0	0.377472	-1.096002	-1.375297
6	1	0	-0.160216	-1.587960	-2.191504
7	6	0	0.520280	-0.851359	1.098326
8	6	0	0.435694	0.549697	1.024922

```
      9          6           0       -0.387386    1.031711   -0.177864
     10          6           0        0.320861    0.442047   -1.471389
     11          1           0       -0.219647    0.794841   -2.354649
     12          6           0        1.253493   -1.451492    2.120121
     13          1           0        1.328761   -2.534872    2.174167
     14          6           0        1.076410    1.352992    1.964652
     15          1           0        1.015763    2.435740    1.898047
     16          6           0        1.803601    0.744067    2.995082
     17          1           0        2.304260    1.362505    3.734812
     18          6           0        1.892393   -0.647841    3.072340
     19          1           0        2.462542   -1.111560    3.872694
     20          6           0       -2.808897   -1.844711    0.052130
     21          1           0       -2.732120   -2.926937    0.129254
     22          6           0       -4.064768   -1.223965    0.025532
     23          1           0       -4.966135   -1.828062    0.084359
     24          6           0       -4.160658    0.165564   -0.073151
     25          1           0       -5.136241    0.643488   -0.090996
     26          6           0       -3.004304    0.953964   -0.146295
     27          1           0       -3.080977    2.035256   -0.219865
     28          6           0        1.854322   -1.433109   -1.508114
     29          6           0        1.783276    0.863461   -1.607637
     30          8           0        2.594987   -0.266606   -1.635785
     31          8           0        2.240483    1.964335   -1.702669
     32          8           0        2.373610   -2.513004   -1.509152
     33          6           0       -0.517241    2.488837   -0.247857
     34          7           0       -0.673093    3.638242   -0.284754
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.3755939      0.2679513
0.2564880
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1879.1549306855 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A)
       Virtual  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1011.11154504     A.U. after   12 cycles
            Convg  =    0.3410D-08             -V/T =  2.0093
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000021311    0.000032398   -0.000010683
      2        6           0.000056220    0.000009133    0.000009120
      3        1          -0.000009473   -0.000000233    0.000005169
```

4	6	-0.000014526	-0.000008012	0.000023416
5	6	0.000038454	-0.000087411	-0.000164788
6	1	-0.000032691	0.000014169	0.000002909
7	6	-0.000014707	-0.000008938	0.000018923
8	6	-0.000009296	0.000005011	0.000005576
9	6	0.000004208	-0.000046236	-0.000035143
10	6	0.000009508	0.000053750	0.000108191
11	1	0.000030193	-0.000002089	-0.000016410
12	6	-0.000011233	-0.000000935	0.000012434
13	1	-0.000000941	0.000002096	0.000002298
14	6	-0.000018315	0.000003795	0.000003957
15	1	0.000005116	0.000000060	0.000003484
16	6	0.000004031	-0.000003533	0.000007353
17	1	-0.000003812	0.000003553	0.000005323
18	6	0.000001602	0.000004146	0.000002118
19	1	-0.000005787	0.000003493	0.000009098
20	6	0.000016454	-0.000014932	-0.000004403
21	1	-0.000002945	0.000001599	-0.000001782
22	6	-0.000009014	0.000013230	-0.000009481
23	1	-0.000002170	0.000001715	-0.000003283
24	6	-0.000009651	-0.000016294	-0.000007025
25	1	-0.000001067	0.000005621	-0.000008667
26	6	0.000034850	0.000009383	-0.000004747
27	1	-0.000003591	0.000004018	-0.000005385
28	6	0.000034804	0.000193889	0.000419210
29	6	-0.000105470	0.000092367	-0.000312028
30	8	0.000035643	-0.000148226	-0.000006397
31	8	0.000009005	-0.000050868	0.000114915
32	8	-0.000000821	-0.000077275	-0.000163347
33	6	0.000002826	0.000022886	0.000013835
34	7	-0.000006093	-0.000011332	-0.000013761

```
 ---------------------------------------------------------------------
 Cartesian Forces:  Max     0.000419210 RMS     0.000068005


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000089845 RMS     0.000020902
 Search for a local minimum.
 Step number   5 out of a maximum of  204
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
 DE= -3.99D-07 DEPred=-2.27D-06 R= 1.75D-01
 Trust test= 1.75D-01 RLast= 1.31D-02 DXMaxT set to 3.00D-01
     Eigenvalues ---    0.00444   0.01043   0.01146   0.01166
0.01422
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---    0.01483   0.01578   0.01817   0.02020
0.02114
     Eigenvalues ---    0.02117   0.02128   0.02129   0.02130
0.02130
     Eigenvalues ---    0.02150   0.02152   0.02158   0.02161
0.02165
     Eigenvalues ---    0.02170   0.02782   0.03820   0.03937
0.04627
     Eigenvalues ---    0.04837   0.04895   0.05041   0.05352
0.05372
     Eigenvalues ---    0.05703   0.06453   0.06779   0.07654
0.08583
     Eigenvalues ---    0.09039   0.09788   0.10119   0.12262
0.15846
     Eigenvalues ---    0.15997   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16000   0.16003   0.16437   0.20482
0.21752
     Eigenvalues ---    0.22000   0.22005   0.22255   0.22596
0.22652
     Eigenvalues ---    0.24413   0.24588   0.24637   0.24759
0.24945
     Eigenvalues ---    0.26378   0.27346   0.27717   0.28792
0.28960
     Eigenvalues ---    0.29378   0.29833   0.34375   0.34410
0.34550
     Eigenvalues ---    0.35129   0.35172   0.35239   0.35251
0.35259
     Eigenvalues ---    0.35265   0.35267   0.35295   0.36504
0.36995
     Eigenvalues ---    0.40065   0.42091   0.42131   0.43442
0.43920
     Eigenvalues ---    0.44167   0.45367   0.45996   0.46132
0.46471
     Eigenvalues ---    0.46516   0.46868   0.47059   1.04265
1.06970
     Eigenvalues ---
1.275501000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     5    4    3    2
1
 RFO step:  Lambda=-3.45537601D-07.
 DIIS coeffs:      0.53529      0.47300     -0.00541     -0.00587
0.00299
 Iteration  1 RMS(Cart)=  0.00034396 RMS(Int)=  0.00000032
 Iteration  2 RMS(Cart)=  0.00000026 RMS(Int)=  0.00000018
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86723   0.00002  -0.00001   0.00006   0.00005
2.86728
    R2        2.65487  -0.00002   0.00006  -0.00014  -0.00008
2.65479
    R3        2.63160   0.00000   0.00005  -0.00007  -0.00002
2.63158
```

This journal is © The Royal Society of Chemistry 2014

R4	2.06454	0.00000	0.00001	-0.00001	0.00000
2.06454					
R5	2.96657	0.00001	0.00003	0.00000	0.00003
2.96660					
R6	2.86944	0.00000	0.00000	0.00002	0.00002
2.86946					
R7	2.91062	-0.00001	0.00001	-0.00003	-0.00002
2.91059					
R8	2.63088	-0.00001	0.00007	-0.00013	-0.00006
2.63082					
R9	2.06778	0.00001	0.00001	0.00000	0.00001
2.06779					
R10	2.91412	0.00002	0.00000	0.00009	0.00008
2.91421					
R11	2.87361	-0.00003	0.00008	-0.00022	-0.00014
2.87346					
R12	2.65606	0.00001	0.00004	-0.00005	-0.00002
2.65604					
R13	2.63332	0.00001	0.00004	-0.00004	0.00000
2.63332					
R14	2.90089	0.00002	0.00006	-0.00007	-0.00001
2.90088					
R15	2.63133	0.00001	0.00005	-0.00005	-0.00001
2.63133					
R16	3.00135	0.00002	0.00009	-0.00010	-0.00001
3.00134					
R17	2.76764	0.00001	0.00001	0.00001	0.00002
2.76766					
R18	2.06730	0.00000	-0.00001	0.00002	0.00001
2.06731					
R19	2.88752	-0.00003	0.00007	-0.00017	-0.00010
2.88742					
R20	2.05477	0.00000	0.00002	-0.00002	-0.00001
2.05476					
R21	2.64614	0.00000	0.00005	-0.00006	-0.00001
2.64613					
R22	2.05317	0.00000	0.00002	-0.00003	-0.00001
2.05315					
R23	2.64655	0.00001	0.00004	-0.00004	0.00000
2.64655					
R24	2.05305	0.00000	0.00001	-0.00001	0.00000
2.05305					
R25	2.63971	0.00000	0.00005	-0.00007	-0.00002
2.63969					
R26	2.05335	0.00000	0.00001	-0.00001	0.00000
2.05335					
R27	2.05543	0.00000	0.00002	-0.00003	-0.00001
2.05542					
R28	2.64781	0.00001	0.00005	-0.00004	0.00000
2.64781					
R29	2.05351	0.00000	0.00001	-0.00001	0.00000
2.05351					

This journal is © The Royal Society of Chemistry 2014

R30	2.63867	0.00000	0.00005	-0.00007	-0.00002
2.63865					
R31	2.05320	0.00000	0.00001	-0.00001	0.00000
2.05320					
R32	2.64837	0.00002	0.00004	-0.00003	0.00001
2.64838					
R33	2.05319	0.00000	0.00001	0.00000	0.00001
2.05320					
R34	2.62231	-0.00008	0.00007	-0.00024	-0.00017
2.62214					
R35	2.26439	0.00007	0.00000	0.00006	0.00006
2.26445					
R36	2.62986	0.00009	-0.00005	0.00022	0.00017
2.63003					
R37	2.25978	-0.00005	0.00003	-0.00008	-0.00005
2.25973					
R38	2.19305	-0.00001	0.00001	-0.00002	-0.00001
2.19304					
A1	1.98460	0.00000	0.00004	-0.00007	-0.00003
1.98457					
A2	2.20282	-0.00001	-0.00002	0.00002	0.00000
2.20282					
A3	2.09567	0.00001	-0.00002	0.00005	0.00003
2.09570					
A4	1.97377	0.00000	0.00002	-0.00012	-0.00010
1.97367					
A5	1.83152	-0.00001	0.00006	-0.00001	0.00005
1.83158					
A6	1.88328	-0.00001	0.00000	-0.00003	-0.00004
1.88325					
A7	1.92659	0.00000	0.00003	-0.00003	-0.00001
1.92658					
A8	1.96605	0.00000	-0.00002	0.00003	0.00000
1.96605					
A9	1.87522	0.00002	-0.00009	0.00019	0.00010
1.87532					
A10	1.97138	0.00000	-0.00001	0.00001	-0.00001
1.97137					
A11	2.10576	0.00001	-0.00001	0.00003	0.00002
2.10579					
A12	2.20604	-0.00001	0.00002	-0.00004	-0.00002
2.20602					
A13	1.90006	0.00000	0.00002	0.00005	0.00007
1.90013					
A14	1.92157	0.00001	0.00004	-0.00014	-0.00009
1.92148					
A15	1.96406	-0.00003	-0.00016	0.00007	-0.00009
1.96397					
A16	1.96481	-0.00002	0.00000	-0.00009	-0.00009
1.96472					
A17	1.88853	0.00003	0.00010	0.00010	0.00020
1.88873					

This journal is © The Royal Society of Chemistry 2014

A18	1.82484	0.00001	0.00000	0.00000	0.00000
1.82484					
A19	1.98942	-0.00001	0.00000	-0.00002	-0.00003
1.98939					
A20	2.20019	0.00001	0.00000	0.00003	0.00002
2.20022					
A21	2.09354	0.00000	0.00001	0.00000	0.00000
2.09354					
A22	1.96729	0.00000	0.00002	-0.00006	-0.00003
1.96726					
A23	2.10845	-0.00001	-0.00001	0.00000	-0.00001
2.10844					
A24	2.20727	0.00001	-0.00002	0.00006	0.00005
2.20731					
A25	1.87794	-0.00001	0.00000	-0.00010	-0.00010
1.87783					
A26	1.83641	0.00001	-0.00013	0.00013	0.00000
1.83641					
A27	1.95442	-0.00001	-0.00001	-0.00011	-0.00012
1.95430					
A28	1.85715	0.00002	0.00008	0.00013	0.00021
1.85736					
A29	1.97946	0.00000	0.00002	-0.00003	0.00000
1.97946					
A30	1.94980	0.00000	0.00003	0.00000	0.00002
1.94982					
A31	1.91337	-0.00002	0.00000	0.00001	0.00001
1.91338					
A32	1.97153	0.00001	0.00001	-0.00012	-0.00011
1.97143					
A33	1.81882	-0.00001	0.00003	-0.00007	-0.00004
1.81878					
A34	1.89390	0.00001	-0.00007	0.00012	0.00005
1.89395					
A35	1.97906	0.00004	0.00020	0.00004	0.00024
1.97930					
A36	1.88803	-0.00003	-0.00017	0.00001	-0.00015
1.88787					
A37	2.09667	0.00000	0.00000	0.00000	0.00000
2.09667					
A38	2.08465	0.00000	0.00000	0.00001	0.00001
2.08466					
A39	2.10186	0.00000	0.00000	-0.00001	-0.00001
2.10186					
A40	2.10349	0.00001	-0.00001	0.00006	0.00004
2.10353					
A41	2.07675	0.00000	0.00001	0.00000	0.00001
2.07676					
A42	2.10294	-0.00001	0.00001	-0.00006	-0.00005
2.10289					
A43	2.08604	0.00000	0.00000	0.00000	0.00000
2.08604					

This journal is © The Royal Society of Chemistry 2014

A44	2.10243	0.00000	-0.00001	0.00001	0.00000
2.10244					
A45	2.09470	0.00000	0.00000	-0.00001	0.00000
2.09470					
A46	2.10049	0.00000	0.00000	-0.00001	-0.00001
2.10048					
A47	2.08905	0.00000	0.00000	0.00002	0.00002
2.08907					
A48	2.09363	0.00000	0.00000	-0.00002	-0.00001
2.09362					
A49	2.09721	0.00000	-0.00001	0.00004	0.00003
2.09724					
A50	2.08531	-0.00001	0.00002	-0.00006	-0.00004
2.08527					
A51	2.10066	0.00000	-0.00001	0.00001	0.00000
2.10066					
A52	2.08996	0.00000	0.00000	0.00000	0.00000
2.08996					
A53	2.09874	0.00000	0.00000	0.00000	0.00000
2.09874					
A54	2.09448	0.00000	0.00000	0.00000	0.00000
2.09448					
A55	2.09504	0.00000	-0.00001	0.00002	0.00002
2.09505					
A56	2.10232	0.00000	-0.00001	0.00002	0.00001
2.10233					
A57	2.08583	0.00000	0.00002	-0.00005	-0.00003
2.08580					
A58	2.07855	0.00000	0.00002	-0.00005	-0.00003
2.07852					
A59	2.10424	0.00001	-0.00001	0.00006	0.00005
2.10429					
A60	2.10037	0.00000	0.00000	-0.00002	-0.00002
2.10035					
A61	1.91777	0.00003	-0.00003	0.00014	0.00011
1.91789					
A62	2.24049	-0.00003	0.00006	-0.00019	-0.00013
2.24036					
A63	2.12492	0.00000	-0.00003	0.00005	0.00002
2.12493					
A64	1.91355	0.00000	-0.00001	0.00005	0.00004
1.91359					
A65	2.24837	0.00002	0.00003	0.00003	0.00006
2.24843					
A66	2.12109	-0.00001	0.00002	-0.00009	-0.00007
2.12103					
A67	1.94919	-0.00002	0.00004	-0.00012	-0.00009
1.94910					
A68	3.09519	-0.00002	0.00034	-0.00108	-0.00074
3.09445					
A69	3.11739	0.00001	-0.00008	0.00033	0.00025
3.11764					

This journal is © The Royal Society of Chemistry 2014

D1	3.13266	0.00000	-0.00010	-0.00013	-0.00023	3.13242
D2	-1.04960	-0.00001	-0.00001	-0.00025	-0.00026	-1.04986
D3	0.94608	0.00001	-0.00008	-0.00005	-0.00014	0.94594
D4	-0.02320	0.00000	0.00005	-0.00015	-0.00010	-0.02331
D5	2.07773	0.00000	0.00014	-0.00027	-0.00013	2.07760
D6	-2.20978	0.00001	0.00007	-0.00007	-0.00001	-2.20979
D7	-0.01188	0.00001	0.00014	0.00021	0.00034	-0.01153
D8	3.12960	0.00000	0.00007	0.00013	0.00020	3.12981
D9	-3.14017	0.00001	0.00000	0.00023	0.00022	-3.13994
D10	0.00131	0.00000	-0.00007	0.00015	0.00008	0.00139
D11	0.01488	0.00000	-0.00008	-0.00006	-0.00014	0.01474
D12	-3.13255	0.00000	-0.00011	-0.00006	-0.00017	-3.13272
D13	3.14138	0.00000	0.00008	-0.00008	0.00000	3.14138
D14	-0.00605	0.00000	0.00004	-0.00008	-0.00004	-0.00609
D15	-1.12008	0.00002	-0.00045	0.00036	-0.00009	-1.12017
D16	1.04152	0.00000	-0.00041	0.00020	-0.00021	1.04131
D17	3.06963	-0.00001	-0.00048	0.00015	-0.00032	3.06931
D18	1.01184	0.00001	-0.00037	0.00018	-0.00018	1.01166
D19	-3.10974	-0.00001	-0.00033	0.00002	-0.00031	-3.11005
D20	-1.08163	-0.00001	-0.00040	-0.00002	-0.00042	-1.08205
D21	-3.12139	0.00002	-0.00043	0.00032	-0.00012	-3.12151
D22	-0.95979	0.00000	-0.00039	0.00015	-0.00024	-0.96003
D23	1.06832	0.00000	-0.00046	0.00011	-0.00035	1.06797
D24	-0.93480	0.00000	-0.00009	-0.00006	-0.00014	-0.93495
D25	2.21519	0.00000	0.00000	-0.00008	-0.00008	2.21511
D26	-3.12596	0.00001	-0.00009	0.00011	0.00001	-3.12595

This journal is © The Royal Society of Chemistry 2014

D27	0.02403	0.00001	-0.00001	0.00009	0.00008	0.02411
D28	1.03170	-0.00001	-0.00006	0.00001	-0.00005	1.03165
D29	-2.10148	-0.00001	0.00003	-0.00001	0.00001	-2.10147
D30	-0.93015	-0.00001	-0.00004	-0.00031	-0.00035	-0.93050
D31	1.04495	0.00001	0.00000	-0.00015	-0.00015	1.04480
D32	-3.11672	0.00000	-0.00006	-0.00013	-0.00019	-3.11691
D33	2.21156	-0.00001	0.00003	-0.00022	-0.00019	2.21137
D34	-2.09652	0.00001	0.00006	-0.00006	0.00000	-2.09652
D35	0.02499	0.00000	0.00001	-0.00004	-0.00004	0.02495
D36	0.00396	0.00000	0.00005	-0.00011	-0.00006	0.00389
D37	3.13765	0.00000	0.00004	-0.00007	-0.00002	3.13763
D38	-3.13777	-0.00001	-0.00002	-0.00020	-0.00023	-3.13799
D39	-0.00407	0.00000	-0.00003	-0.00016	-0.00019	-0.00425
D40	-0.04040	-0.00001	0.00056	-0.00017	0.00039	-0.04001
D41	-2.15478	-0.00001	0.00064	-0.00024	0.00040	-2.15438
D42	2.08326	0.00003	0.00081	-0.00016	0.00066	2.08392
D43	2.08313	-0.00001	0.00061	-0.00026	0.00035	2.08348
D44	-0.03125	-0.00002	0.00069	-0.00033	0.00036	-0.03089
D45	-2.07639	0.00002	0.00087	-0.00024	0.00062	-2.07577
D46	-2.15407	0.00002	0.00073	-0.00018	0.00055	-2.15352
D47	2.01474	0.00002	0.00081	-0.00026	0.00055	2.01530
D48	-0.03040	0.00006	0.00098	-0.00017	0.00082	-0.02959
D49	-2.06433	-0.00005	-0.00107	0.00064	-0.00042	-2.06476
D50	1.07545	0.00008	0.00191	0.00085	0.00276	1.07821
D51	2.11872	-0.00005	-0.00105	0.00047	-0.00059	2.11813
D52	-1.02468	0.00007	0.00193	0.00067	0.00260	-1.02209

This journal is © The Royal Society of Chemistry 2014

D53	0.02095	-0.00005	-0.00110	0.00052	-0.00058	0.02037
D54	-3.12245	0.00007	0.00188	0.00072	0.00260	-3.11985
D55	-0.01222	0.00000	0.00018	-0.00004	0.00014	-0.01208
D56	-3.13495	0.00000	0.00006	-0.00007	-0.00001	-3.13496
D57	3.12154	0.00000	0.00010	-0.00002	0.00008	3.12162
D58	-0.00120	0.00000	-0.00002	-0.00005	-0.00007	-0.00127
D59	0.00137	0.00000	-0.00007	0.00010	0.00003	0.00140
D60	3.14101	0.00000	-0.00005	-0.00010	-0.00015	3.14087
D61	-3.13136	0.00000	0.00002	0.00008	0.00010	-3.13126
D62	0.00829	0.00000	0.00004	-0.00012	-0.00008	0.00820
D63	0.94159	0.00001	-0.00013	0.00019	0.00006	0.94165
D64	-1.01951	0.00000	-0.00002	0.00003	0.00001	-1.01951
D65	3.11312	-0.00001	-0.00013	-0.00005	-0.00017	3.11294
D66	-2.22014	0.00001	0.00000	0.00022	0.00022	-2.21993
D67	2.10194	0.00000	0.00011	0.00006	0.00016	2.10211
D68	-0.04861	-0.00001	0.00000	-0.00002	-0.00001	-0.04863
D69	3.13140	0.00000	0.00008	-0.00011	-0.00004	3.13136
D70	-0.00703	0.00000	0.00000	0.00017	0.00017	-0.00686
D71	0.01144	0.00000	-0.00006	-0.00015	-0.00021	0.01123
D72	-3.12699	0.00000	-0.00014	0.00014	0.00000	-3.12699
D73	-0.97445	0.00000	-0.00041	0.00013	-0.00028	-0.97473
D74	1.18612	0.00000	-0.00044	0.00006	-0.00037	1.18575
D75	-2.99890	0.00000	-0.00057	0.00019	-0.00038	-2.99928
D76	1.01521	0.00000	-0.00043	0.00013	-0.00030	1.01491
D77	-3.10740	0.00000	-0.00046	0.00006	-0.00040	-3.10780
D78	-1.00924	0.00000	-0.00058	0.00018	-0.00040	-1.00964

This journal is © The Royal Society of Chemistry 2014

D79	-3.09897	0.00001	-0.00032	0.00018	-0.00014	-3.09912
D80	-0.93839	0.00001	-0.00035	0.00011	-0.00024	-0.93863
D81	1.15977	0.00001	-0.00048	0.00024	-0.00025	1.15952
D82	0.03149	-0.00005	-0.00060	-0.00023	-0.00083	0.03067
D83	-3.13009	0.00004	0.00138	-0.00004	0.00134	-3.12876
D84	2.11105	-0.00005	-0.00048	-0.00024	-0.00071	2.11034
D85	-1.05054	0.00004	0.00150	-0.00006	0.00145	-1.04909
D86	-2.07064	-0.00003	-0.00055	-0.00006	-0.00061	-2.07125
D87	1.05096	0.00006	0.00143	0.00013	0.00156	1.05251
D88	-0.00714	0.00000	-0.00004	0.00017	0.00013	-0.00701
D89	3.13816	0.00000	0.00002	0.00002	0.00004	3.13820
D90	3.13250	0.00000	-0.00002	-0.00003	-0.00005	3.13245
D91	-0.00539	0.00000	0.00004	-0.00018	-0.00014	-0.00553
D92	-3.13819	0.00000	0.00000	-0.00009	-0.00009	-3.13828
D93	0.00819	0.00000	0.00000	-0.00012	-0.00012	0.00807
D94	0.00657	0.00000	-0.00008	0.00019	0.00011	0.00668
D95	-3.13024	0.00000	-0.00008	0.00016	0.00009	-3.13016
D96	-0.00115	0.00000	0.00002	-0.00005	-0.00003	-0.00118
D97	3.13673	0.00000	-0.00005	0.00011	0.00006	3.13679
D98	-3.13794	0.00000	0.00002	-0.00008	-0.00006	-3.13799
D99	-0.00006	0.00000	-0.00004	0.00008	0.00004	-0.00002
D100	-3.13360	0.00000	-0.00002	0.00009	0.00007	-3.13352
D101	0.00553	0.00000	-0.00001	-0.00002	-0.00003	0.00550
D102	0.00215	0.00000	-0.00005	0.00009	0.00004	0.00219
D103	3.14128	0.00000	-0.00004	-0.00002	-0.00006	3.14122
D104	-3.13893	0.00000	-0.00001	0.00005	0.00004	-3.13889

```
   D105      -0.00025   0.00000  -0.00001   0.00005   0.00004  -
0.00020
   D106       0.00019   0.00000   0.00000  -0.00006  -0.00006
0.00013
   D107       3.13887   0.00000   0.00000  -0.00006  -0.00006
3.13882
   D108      -0.00448   0.00000  -0.00001   0.00001   0.00000  -
0.00448
   D109      -3.13820   0.00000  -0.00001  -0.00003  -0.00004  -
3.13824
   D110       3.13422   0.00000  -0.00001   0.00001   0.00000
3.13422
   D111       0.00050   0.00000  -0.00001  -0.00003  -0.00004
0.00046
   D112      -0.00127   0.00003   0.00077  -0.00070   0.00007  -
0.00121
   D113      -3.14120  -0.00009  -0.00198  -0.00089  -0.00287
3.13912
   D114      -0.01969   0.00001  -0.00009   0.00058   0.00049  -
0.01920
   D115       3.14018  -0.00007  -0.00190   0.00041  -0.00148
3.13869
         Item               Value     Threshold  Converged?
 Maximum Force            0.000090     0.000450     YES
 RMS     Force            0.000021     0.000300     YES
 Maximum Displacement     0.003018     0.001800     NO
 RMS     Displacement     0.000344     0.001200     YES
 Predicted change in Energy=-7.799012D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.657134   -1.063444   -0.025040
      2          6           0       -0.228244   -1.573561   -0.040814
      3          1           0       -0.161299   -2.662083    0.024050
      4          6           0       -1.758123    0.335970   -0.096116
      5          6           0        0.366526   -1.069346   -1.403336
      6          1           0       -0.178057   -1.544796   -2.224746
      7          6           0        0.529531   -0.873745    1.073519
      8          6           0        0.445541    0.528538    1.028489
      9          6           0       -0.386917    1.034733   -0.157789
     10          6           0        0.310029    0.470367   -1.468618
     11          1           0       -0.237732    0.840633   -2.340190
     12          6           0        1.270463   -1.494455    2.077293
     13          1           0        1.345318   -2.578736    2.109262
     14          6           0        1.094444    1.312651    1.978740
     15          1           0        1.034241    2.396544    1.934055
```

This journal is © The Royal Society of Chemistry 2014

16	6	0	1.829517	0.682983	2.990951
17	1	0	2.336681	1.286338	3.738664
18	6	0	1.917796	-0.710225	3.039944
19	1	0	2.494031	-1.190049	3.826325
20	6	0	-2.808772	-1.844084	0.034865
21	1	0	-2.732252	-2.927681	0.089724
22	6	0	-4.064309	-1.222101	0.031011
23	1	0	-4.965660	-1.826653	0.085218
24	6	0	-4.159856	0.169177	-0.039032
25	1	0	-5.135149	0.648026	-0.039254
26	6	0	-3.003494	0.958133	-0.105912
27	1	0	-3.079911	2.040731	-0.157217
28	6	0	1.842016	-1.404362	-1.554441
29	6	0	1.771429	0.893655	-1.609278
30	8	0	2.582319	-0.236056	-1.665684
31	8	0	2.228681	1.995956	-1.685355
32	8	0	2.360274	-2.484402	-1.583303
33	6	0	-0.516317	2.493040	-0.197843
34	7	0	-0.672509	3.642913	-0.210815

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.517299	0.000000			
3	H	2.189881	1.092506	0.000000		
4	C	1.404853	2.447426	3.398913	0.000000	
5	C	2.448456	1.569857	2.202917	2.863192	0.000000
6	H	2.694081	2.184698	2.511114	3.250377	1.094229
7	C	2.454450	1.518455	2.185586	2.839862	2.489909
8	C	2.839996	2.452797	3.399590	2.481522	2.910885
9	C	2.456303	2.615733	3.708156	1.540220	2.558557
10	C	2.882052	2.550686	3.501778	2.485775	1.542131
11	H	3.316644	3.333999	4.226640	2.757198	2.211524
12	C	3.629931	2.595912	2.762083	4.152890	3.621133
13	H	3.983224	2.847683	2.573898	4.794846	3.946472
14	C	4.151162	3.762754	4.603934	3.660064	4.200263
15	H	4.801361	4.610391	5.537792	4.020553	4.857614
16	C	4.929802	4.303251	4.894417	4.745688	4.951844
17	H	5.969716	5.389093	5.968944	5.690005	5.989234
18	C	4.722184	3.852520	4.150663	4.943863	4.719974
19	H	5.664029	4.744748	4.865692	5.982900	5.647142
20	C	1.392572	2.595772	2.770984	2.423563	3.570877
21	H	2.155093	2.849690	2.585469	3.410994	3.909611
22	C	2.413049	3.852801	4.160178	2.786080	4.659720
23	H	3.397202	4.745845	4.876839	3.872740	5.587622
24	C	2.789833	4.300548	4.899843	2.408195	4.887065
25	H	3.876328	5.386387	5.974948	3.391890	5.922712
26	C	2.430226	3.757089	4.604446	1.392168	4.141378
27	H	3.417260	4.605286	5.537834	2.158024	4.806591
28	C	3.833972	2.570150	2.843724	4.256344	1.520572
29	C	4.253833	3.542023	4.364226	3.880517	2.422712
30	O	4.620525	3.511180	4.033392	4.650827	2.381793

31	O	5.216909	4.634916	5.507395	4.601721	3.597670
32	O	4.537276	3.147909	2.995578	5.208398	2.451490
33	C	3.738972	4.079815	5.172095	2.491060	3.863058
34	N	4.811839	5.238117	6.330045	3.482468	4.970621
		6	7	8	9	10
6	H	0.000000				
7	C	3.439410	0.000000			
8	C	3.907829	1.405517	0.000000		
9	C	3.312085	2.449139	1.535082	0.000000	
10	C	2.206998	2.883969	2.501458	1.588243	0.000000
11	H	2.388966	3.896305	3.451415	2.196088	1.093973
12	C	4.539635	1.393493	2.423424	3.760225	4.166106
13	H	4.708856	2.155288	3.410692	4.604054	4.813530
14	C	5.239614	2.432874	1.392438	2.614655	3.634422
15	H	5.856573	3.419070	2.157791	2.872286	3.976533
16	C	6.016381	2.791041	2.406345	3.866635	4.716121
17	H	7.064099	3.877467	3.390534	4.760634	5.647027
18	C	5.727659	2.412643	2.783526	4.310694	4.930095
19	H	6.624301	3.396653	3.870108	5.396544	5.963494
20	C	3.480815	3.628309	4.148153	3.766973	4.164621
21	H	3.713899	3.978157	4.788015	4.611137	4.819816
22	C	4.505055	4.723509	4.939478	4.318815	4.924243
23	H	5.323205	5.664088	5.976435	5.404764	5.960168
24	C	4.854871	4.931105	4.741142	3.872772	4.702585
25	H	5.844450	5.970146	5.683173	4.765428	5.632460
26	C	4.328649	4.150794	3.656126	2.618212	3.615843
27	H	5.054843	4.799682	4.015151	2.874761	3.959484
28	C	2.133009	2.985021	3.515363	3.587195	2.422593
29	C	3.182034	3.444331	2.974745	2.604838	1.527955
30	O	3.105645	3.481928	3.522640	3.564409	2.387712
31	O	4.315119	4.328242	3.563405	3.177854	2.460817
32	O	2.781624	3.606181	4.423287	4.686519	3.598238
33	C	4.530660	3.747719	2.507655	1.464584	2.527632
34	N	5.586835	4.847123	3.533446	2.624304	3.551407
		11	12	13	14	15
11	H	0.000000				
12	C	5.219333	0.000000			
13	H	5.830587	1.087332	0.000000		
14	C	4.544298	2.814346	3.901649	0.000000	
15	H	4.723128	3.900793	4.988073	1.086482	0.000000
16	C	5.720090	2.426633	3.413303	1.400495	2.164667
17	H	6.616549	3.410247	4.310052	2.154340	2.487071
18	C	5.999775	1.400270	2.164540	2.428187	3.414041
19	H	7.043586	2.156130	2.489237	3.411147	4.309910
20	C	4.411217	4.575359	4.700989	5.383189	6.029809
21	H	5.131013	4.693217	4.563647	6.016011	6.777565
22	C	4.951783	5.720248	5.951777	6.068884	6.535394
23	H	5.945613	6.554993	6.670144	7.082761	7.566531
24	C	4.596655	6.060929	6.517141	5.743396	5.986057
25	H	5.414434	7.078267	7.551461	6.581934	6.709145
26	C	3.557420	5.389645	6.027321	4.611350	4.746977
27	H	3.779363	6.034594	6.786682	4.745276	4.628851

This journal is © The Royal Society of Chemistry 2014

28	C	3.159550	3.677538	3.879250	4.519335	5.221972
29	C	2.138638	4.420955	5.105547	3.675288	3.918843
30	O	3.093041	4.161059	4.611782	4.230140	4.720725
31	O	2.801209	5.220984	6.008931	3.896022	3.832400
32	O	4.287000	3.945585	3.830674	5.357993	6.160666
33	C	2.719873	4.926352	5.874634	2.953875	2.637902
34	N	3.546271	5.950052	6.939978	3.653271	3.011129
		16	17	18	19	20
16	C	0.000000				
17	H	1.086429	0.000000			
18	C	1.396862	2.156371	0.000000		
19	H	2.155848	2.482929	1.086588	0.000000	
20	C	6.052953	7.070598	5.714594	6.551539	0.000000
21	H	6.501057	7.534374	5.936654	6.655493	1.087679
22	C	6.864967	7.810995	6.715749	7.577418	1.401161
23	H	7.804869	8.738568	7.573558	8.369476	2.157546
24	C	6.731818	7.597633	6.869592	7.814262	2.425718
25	H	7.595389	8.396925	7.814752	8.747892	3.410005
26	C	5.746674	6.588320	6.074449	7.092246	2.812499
27	H	5.988064	6.714646	6.539623	7.574653	3.899000
28	C	5.001775	5.958316	4.647144	5.424362	4.934478
29	C	4.605417	5.392050	4.920277	5.865983	5.583607
30	O	4.805787	5.620053	4.775915	5.574950	5.877200
31	O	4.873507	5.471308	5.454220	6.371786	6.563611
32	O	5.589081	6.522451	4.971710	5.563930	5.454127
33	C	4.352889	5.009173	5.164211	6.230672	4.911227
34	N	5.027188	5.496095	6.018880	7.048617	5.893311
		21	22	23	24	25
21	H	0.000000				
22	C	2.164908	0.000000			
23	H	2.490059	1.086671	0.000000		
24	C	3.412500	1.396312	2.155944	0.000000	
25	H	4.310015	2.156156	2.483598	1.086505	0.000000
26	C	3.900178	2.428476	3.411987	1.401463	2.155125
27	H	4.986678	3.413289	4.309465	2.164016	2.485467
28	C	5.093888	6.118133	7.015074	6.387093	7.428924
29	C	6.145922	6.420500	7.460547	6.178243	7.087040
30	O	6.210552	6.930276	7.909971	6.947455	7.936384
31	O	7.211377	7.273481	8.337014	6.845503	7.665021
32	O	5.378599	6.743492	7.542274	7.206826	8.269072
33	C	5.863214	5.142266	6.207780	4.324459	4.976227
34	N	6.892428	5.935583	6.959521	4.925236	5.377168
		26	27	28	29	30
26	C	0.000000				
27	H	1.086504	0.000000			
28	C	5.581987	6.168166	0.000000		
29	C	5.006412	5.192280	2.299755	0.000000	
30	O	5.921172	6.286500	1.387575	1.391751	0.000000
31	O	5.563036	5.524342	3.424736	1.195799	2.259939
32	O	6.542456	7.218460	1.198295	3.429094	2.260786
33	C	2.924114	2.603507	4.753087	3.127933	4.382244
34	N	3.557041	2.892308	5.796822	3.935346	5.268486

This journal is © The Royal Society of Chemistry 2014

```
                31         32         33         34
   31  O    0.000000
   32  O    4.483452   0.000000
   33  C    3.161455   5.913477   0.000000
   34  N    3.647415   6.973197   1.160505   0.000000
Stoichiometry    C19H11NO3
Framework group  C1[X(C19H11NO3)]
Deg. of freedom    96
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                      Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -1.657079   -1.064686   -0.013600
     2          6           0       -0.227741   -1.573747   -0.007070
     3          1           0       -0.160558   -2.660664    0.080496
     4          6           0       -1.758476    0.332902   -0.113989
     5          6           0        0.378031   -1.096836   -1.374568
     6          1           0       -0.159329   -1.589388   -2.190641
     7          6           0        0.520194   -0.850726    1.099066
     8          6           0        0.435575    0.550275    1.024800
     9          6           0       -0.387305    1.031484   -0.178438
    10          6           0        0.320974    0.441178   -1.471648
    11          1           0       -0.219752    0.793143   -2.355115
    12          6           0        1.253159   -1.450221    2.121412
    13          1           0        1.328524   -2.533560    2.176070
    14          6           0        1.075952    1.354140    1.964269
    15          1           0        1.015345    2.436845    1.897028
    16          6           0        1.802994    0.745856    2.995183
    17          1           0        2.303460    1.364752    3.734663
    18          6           0        1.891863   -0.645988    3.073263
    19          1           0        2.461852   -1.109198    3.874027
    20          6           0       -2.808616   -1.844968    0.052578
    21          1           0       -2.731777   -2.927155    0.130121
    22          6           0       -4.064523   -1.224308    0.025594
    23          1           0       -4.965861   -1.828433    0.084579
    24          6           0       -4.160482    0.165170   -0.073551
    25          1           0       -5.136083    0.643049   -0.091655
    26          6           0       -3.004169    0.953629   -0.146834
    27          1           0       -3.080933    2.034891   -0.220802
    28          6           0        1.854972   -1.433547   -1.506512
    29          6           0        1.783194    0.862815   -1.608705
    30          8           0        2.595339   -0.267089   -1.635338
    31          8           0        2.240273    1.963745   -1.703391
    32          8           0        2.374229   -2.513490   -1.509058
    33          6           0       -0.517415    2.488558   -0.249248
    34          7           0       -0.674319    3.637789   -0.286928
---------------------------------------------------------------------
```

This journal is © The Royal Society of Chemistry 2014

```
 Rotational constants (GHZ):      0.3755593      0.2679362
0.2565006
 Standard basis: 6-31+G(d) (6D, 7F)
 There are   459 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   459 basis functions,   780 primitive gaussians,   459 cartesian
basis functions
    78 alpha electrons       78 beta electrons
       nuclear repulsion energy      1879.1394801088 Hartrees.
 NAtoms=   34 NActive=   34 NUniq=   34 SFac= 7.50D-01 NAtFMM=   80
NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=   459 RedAO= T  NBF=   459
 NBsUse=   454 1.00D-06 NBFU=   454
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=
0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

This journal is © The Royal Society of Chemistry 2014

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -1011.11154609     A.U. after   12 cycles
            Convg  =    0.1911D-08             -V/T =  2.0093
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0
NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6           0.000003307   -0.000000186    0.000001978
      2          6           0.000013207   -0.000000357    0.000001638
      3          1          -0.000001987   -0.000003120    0.000004492
      4          6          -0.000004826    0.000009516   -0.000005266
      5          6           0.000007048   -0.000037805   -0.000010259
      6          1           0.000001610   -0.000003744    0.000009399
      7          6          -0.000006144   -0.000011991   -0.000000575
      8          6          -0.000005881    0.000001836   -0.000003912
      9          6           0.000036856   -0.000002918   -0.000014325
     10          6           0.000000488    0.000016935    0.000010953
     11          1           0.000005233   -0.000003577   -0.000002172
     12          6          -0.000001013   -0.000007730   -0.000000810
     13          1          -0.000004480   -0.000002139    0.000005601
     14          6           0.000000366    0.000006156   -0.000003877
     15          1          -0.000002019    0.000004616    0.000001575
     16          6          -0.000001554    0.000004448    0.000009448
     17          1          -0.000003954    0.000003982    0.000004510
     18          6          -0.000004733   -0.000000238    0.000011629
     19          1          -0.000004709    0.000001655    0.000007042
     20          6           0.000006833   -0.000010153   -0.000000707
     21          1          -0.000001423   -0.000001021   -0.000001144
     22          6          -0.000010287    0.000003840   -0.000004721
     23          1          -0.000003085    0.000000909   -0.000006925
     24          6          -0.000011247   -0.000003046   -0.000004517
     25          1          -0.000001804    0.000003506   -0.000008281
     26          6           0.000002603    0.000016176   -0.000010505
     27          1          -0.000000543   -0.000000331   -0.000006838
     28          6           0.000019462    0.000093746   -0.000005844
     29          6          -0.000040146    0.000069923    0.000004463
     30          8           0.000011102   -0.000091553    0.000016316
```

```
     31        8           0.000006110   -0.000020667    0.000001858
     32        8           0.000009388   -0.000047460    0.000005601
     33        6          -0.000031610    0.000003683    0.000004637
     34        7           0.000017833    0.000007106   -0.000010461
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000093746 RMS     0.000018465


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000058681 RMS     0.000007812
 Search for a local minimum.
 Step number   6 out of a maximum of  204
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    1    2    3    4
5
                                                      6
 DE= -1.05D-06 DEPred=-7.80D-07 R= 1.34D+00
 SS=  1.41D+00  RLast= 6.85D-03 DXNew= 5.0454D-01 2.0561D-02
 Trust test= 1.34D+00 RLast= 6.85D-03 DXMaxT set to 3.00D-01
     Eigenvalues ---    0.00440   0.00990   0.01147   0.01166
0.01427
     Eigenvalues ---    0.01486   0.01580   0.01818   0.02012
0.02113
     Eigenvalues ---    0.02117   0.02129   0.02129   0.02130
0.02130
     Eigenvalues ---    0.02150   0.02153   0.02160   0.02163
0.02167
     Eigenvalues ---    0.02173   0.02784   0.03825   0.03947
0.04744
     Eigenvalues ---    0.04774   0.04888   0.05308   0.05380
0.05498
     Eigenvalues ---    0.05647   0.06518   0.06809   0.07712
0.08595
     Eigenvalues ---    0.09105   0.09818   0.10140   0.12245
0.15793
     Eigenvalues ---    0.15998   0.16000   0.16000   0.16000
0.16000
     Eigenvalues ---    0.16001   0.16003   0.16433   0.20473
0.21474
     Eigenvalues ---    0.22000   0.22006   0.22219   0.22597
0.22658
     Eigenvalues ---    0.24414   0.24533   0.24590   0.24766
0.24831
     Eigenvalues ---    0.26404   0.27493   0.27734   0.28582
0.28868
     Eigenvalues ---    0.29247   0.29876   0.34382   0.34409
0.34555
```

```
     Eigenvalues ---    0.35138   0.35184   0.35240   0.35252
0.35260
     Eigenvalues ---    0.35267   0.35280   0.35323   0.36509
0.36955
     Eigenvalues ---    0.40087   0.42097   0.42127   0.42465
0.43640
     Eigenvalues ---    0.44190   0.45088   0.46008   0.46134
0.46479
     Eigenvalues ---    0.46534   0.46954   0.49116   1.04262
1.06590
     Eigenvalues ---
1.276171000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
```

This journal is © The Royal Society of Chemistry 2014

```
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues ---
1000.000001000.000001000.000001000.000001000.00000
     Eigenvalues --- 1000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     6    5    4    3
2
 RFO step:  Lambda=-2.57086221D-08.
 DIIS coeffs:      0.89498      0.04837      0.06038     -0.00034
-0.00340
 Iteration  1 RMS(Cart)=  0.00013374 RMS(Int)=  0.00000009
 Iteration  2 RMS(Cart)=  0.00000003 RMS(Int)=  0.00000009
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New
X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.86728   0.00001   0.00000   0.00005   0.00004
2.86732
    R2        2.65479   0.00002   0.00002   0.00000   0.00002
2.65480
    R3        2.63158   0.00001   0.00001   0.00000   0.00001
2.63159
    R4        2.06454   0.00000   0.00000   0.00001   0.00001
2.06454
    R5        2.96660   0.00000   0.00000   0.00000   0.00000
2.96660
    R6        2.86946   0.00000   0.00000  -0.00002  -0.00002
2.86944
    R7        2.91059   0.00001   0.00001   0.00004   0.00004
2.91064
    R8        2.63082   0.00001   0.00002   0.00000   0.00002
2.63083
    R9        2.06779   0.00000   0.00000  -0.00001  -0.00001
2.06778
   R10        2.91421   0.00002  -0.00001   0.00010   0.00010
2.91430
   R11        2.87346   0.00000   0.00002  -0.00007  -0.00005
2.87342
   R12        2.65604   0.00001   0.00001   0.00002   0.00003
2.65607
   R13        2.63332   0.00001   0.00001   0.00001   0.00001
2.63333
   R14        2.90088   0.00001   0.00001   0.00002   0.00002
2.90091
   R15        2.63133   0.00001   0.00001   0.00001   0.00002
2.63134
   R16        3.00134  -0.00001   0.00001  -0.00007  -0.00006
3.00128
```

This journal is © The Royal Society of Chemistry 2014

R17	2.76766	0.00001	0.00000	0.00003	0.00003
2.76770					
R18	2.06731	0.00000	0.00000	0.00001	0.00001
2.06732					
R19	2.88742	-0.00001	0.00002	-0.00006	-0.00004
2.88738					
R20	2.05476	0.00000	0.00000	0.00000	0.00001
2.05477					
R21	2.64613	0.00001	0.00001	0.00001	0.00002
2.64614					
R22	2.05315	0.00000	0.00000	0.00000	0.00001
2.05316					
R23	2.64655	0.00001	0.00001	0.00001	0.00002
2.64657					
R24	2.05305	0.00000	0.00000	0.00000	0.00001
2.05306					
R25	2.63969	0.00001	0.00001	0.00000	0.00001
2.63970					
R26	2.05335	0.00000	0.00000	0.00000	0.00001
2.05336					
R27	2.05542	0.00000	0.00000	0.00000	0.00000
2.05542					
R28	2.64781	0.00002	0.00001	0.00002	0.00003
2.64784					
R29	2.05351	0.00000	0.00000	0.00000	0.00001
2.05352					
R30	2.63865	0.00001	0.00001	0.00000	0.00001
2.63865					
R31	2.05320	0.00000	0.00000	0.00001	0.00001
2.05320					
R32	2.64838	0.00002	0.00001	0.00003	0.00003
2.64842					
R33	2.05320	0.00000	0.00000	0.00000	0.00000
2.05319					
R34	2.62214	-0.00005	0.00003	-0.00015	-0.00012
2.62201					
R35	2.26445	0.00004	0.00000	0.00006	0.00005
2.26450					
R36	2.63003	0.00006	-0.00002	0.00017	0.00015
2.63018					
R37	2.25973	-0.00002	0.00001	-0.00003	-0.00002
2.25971					
R38	2.19304	0.00001	0.00000	0.00000	0.00000
2.19304					
A1	1.98457	0.00000	0.00001	0.00001	0.00002
1.98459					
A2	2.20282	0.00000	0.00000	-0.00002	-0.00002
2.20280					
A3	2.09570	0.00000	0.00000	0.00001	0.00001
2.09571					
A4	1.97367	0.00000	0.00001	-0.00004	-0.00003
1.97364					

This journal is © The Royal Society of Chemistry 2014

A5	1.83158	0.00000	0.00000	-0.00001	-0.00001
1.83156					
A6	1.88325	0.00000	0.00000	-0.00003	-0.00002
1.88322					
A7	1.92658	0.00000	0.00001	0.00001	0.00002
1.92660					
A8	1.96605	0.00000	0.00000	0.00000	0.00000
1.96605					
A9	1.87532	0.00000	-0.00002	0.00007	0.00005
1.87537					
A10	1.97137	-0.00001	0.00000	-0.00002	-0.00002
1.97135					
A11	2.10579	0.00000	0.00000	0.00001	0.00000
2.10579					
A12	2.20602	0.00001	0.00001	0.00002	0.00002
2.20605					
A13	1.90013	0.00000	-0.00001	-0.00003	-0.00004
1.90010					
A14	1.92148	0.00000	0.00001	-0.00005	-0.00004
1.92144					
A15	1.96397	0.00000	-0.00001	0.00003	0.00003
1.96400					
A16	1.96472	0.00000	0.00001	0.00001	0.00002
1.96474					
A17	1.88873	0.00000	-0.00001	0.00005	0.00004
1.88877					
A18	1.82484	0.00000	0.00000	-0.00001	-0.00001
1.82483					
A19	1.98939	0.00000	0.00000	-0.00001	-0.00001
1.98939					
A20	2.20022	0.00000	0.00000	0.00000	-0.00001
2.20021					
A21	2.09354	0.00000	0.00000	0.00001	0.00001
2.09356					
A22	1.96726	0.00000	0.00001	0.00000	0.00001
1.96727					
A23	2.10844	0.00000	0.00000	-0.00001	-0.00001
2.10843					
A24	2.20731	0.00000	-0.00001	0.00001	0.00000
2.20732					
A25	1.87783	0.00000	0.00001	-0.00002	-0.00001
1.87783					
A26	1.83641	0.00000	-0.00002	0.00002	0.00000
1.83641					
A27	1.95430	0.00000	0.00001	-0.00005	-0.00003
1.95426					
A28	1.85736	0.00000	-0.00001	0.00002	0.00001
1.85737					
A29	1.97946	0.00000	0.00000	0.00003	0.00003
1.97950					
A30	1.94982	0.00000	0.00000	0.00000	0.00000
1.94982					

This journal is © The Royal Society of Chemistry 2014

A31	1.91338	0.00000	0.00000	0.00002	0.00002
1.91340					
A32	1.97143	0.00000	0.00001	-0.00003	-0.00002
1.97141					
A33	1.81878	0.00000	0.00001	-0.00002	-0.00001
1.81877					
A34	1.89395	0.00000	-0.00002	0.00004	0.00003
1.89398					
A35	1.97930	0.00000	0.00001	-0.00003	-0.00002
1.97928					
A36	1.88787	0.00000	-0.00001	0.00001	0.00000
1.88788					
A37	2.09667	0.00000	0.00000	0.00000	0.00001
2.09668					
A38	2.08466	0.00000	0.00000	-0.00001	-0.00001
2.08465					
A39	2.10186	0.00000	0.00000	0.00000	0.00000
2.10186					
A40	2.10353	0.00000	0.00000	0.00002	0.00002
2.10355					
A41	2.07676	0.00000	0.00000	0.00000	0.00000
2.07676					
A42	2.10289	0.00000	0.00000	-0.00003	-0.00002
2.10287					
A43	2.08604	0.00000	0.00000	-0.00001	0.00000
2.08604					
A44	2.10244	0.00000	0.00000	0.00000	0.00000
2.10244					
A45	2.09470	0.00000	0.00000	0.00000	0.00000
2.09470					
A46	2.10048	0.00000	0.00000	0.00000	0.00000
2.10048					
A47	2.08907	0.00000	0.00000	0.00001	0.00001
2.08908					
A48	2.09362	0.00000	0.00000	-0.00001	0.00000
2.09362					
A49	2.09724	0.00000	0.00000	0.00001	0.00001
2.09725					
A50	2.08527	0.00000	0.00001	-0.00001	-0.00001
2.08526					
A51	2.10066	0.00000	0.00000	0.00000	0.00000
2.10066					
A52	2.08996	0.00000	0.00000	0.00000	0.00000
2.08996					
A53	2.09874	0.00000	0.00000	0.00000	0.00000
2.09874					
A54	2.09448	0.00000	0.00000	0.00000	0.00000
2.09448					
A55	2.09505	0.00000	0.00000	0.00001	0.00000
2.09506					
A56	2.10233	0.00000	0.00000	0.00001	0.00000
2.10233					

This journal is © The Royal Society of Chemistry 2014

A57	2.08580	0.00000	0.00000	-0.00001	-0.00001
2.08579					
A58	2.07852	0.00000	0.00001	-0.00001	-0.00001
2.07851					
A59	2.10429	0.00000	0.00000	0.00003	0.00003
2.10432					
A60	2.10035	0.00000	0.00000	-0.00002	-0.00002
2.10033					
A61	1.91789	0.00001	-0.00001	0.00006	0.00005
1.91794					
A62	2.24036	-0.00002	0.00002	-0.00011	-0.00009
2.24028					
A63	2.12493	0.00001	-0.00001	0.00004	0.00004
2.12497					
A64	1.91359	-0.00001	-0.00001	-0.00001	-0.00002
1.91357					
A65	2.24843	0.00002	0.00000	0.00006	0.00006
2.24849					
A66	2.12103	0.00000	0.00001	-0.00005	-0.00004
2.12099					
A67	1.94910	0.00000	0.00001	-0.00002	-0.00001
1.94910					
A68	3.09445	0.00004	0.00013	0.00046	0.00059
3.09504					
A69	3.11764	0.00001	-0.00003	0.00022	0.00019
3.11783					
D1	3.13242	0.00000	0.00001	0.00003	0.00004
3.13246					
D2	-1.04986	0.00000	0.00003	0.00001	0.00004	-
1.04982					
D3	0.94594	0.00000	0.00000	0.00008	0.00008
0.94602					
D4	-0.02331	0.00000	0.00002	-0.00002	0.00000	-
0.02331					
D5	2.07760	0.00000	0.00003	-0.00004	0.00000
2.07759					
D6	-2.20979	0.00000	0.00001	0.00003	0.00004	-
2.20975					
D7	-0.01153	0.00000	-0.00002	-0.00007	-0.00009	-
0.01162					
D8	3.12981	0.00000	-0.00001	-0.00005	-0.00006
3.12974					
D9	-3.13994	0.00000	-0.00003	-0.00003	-0.00005	-
3.14000					
D10	0.00139	0.00000	-0.00002	-0.00001	-0.00003
0.00137					
D11	0.01474	0.00000	0.00000	0.00002	0.00003
0.01477					
D12	-3.13272	0.00000	0.00000	0.00004	0.00004	-
3.13268					
D13	3.14138	0.00000	0.00001	-0.00003	-0.00002
3.14136					

This journal is © The Royal Society of Chemistry 2014

D14	-0.00609	0.00000	0.00001	-0.00001	0.00000	-0.00609
D15	-1.12017	0.00000	-0.00005	0.00013	0.00009	-1.12008
D16	1.04131	0.00000	-0.00003	0.00009	0.00006	1.04137
D17	3.06931	0.00000	-0.00002	0.00006	0.00004	3.06934
D18	1.01166	0.00000	-0.00003	0.00008	0.00005	1.01171
D19	-3.11005	0.00000	-0.00001	0.00004	0.00003	-3.11002
D20	-1.08205	0.00000	-0.00001	0.00001	0.00001	-1.08205
D21	-3.12151	0.00000	-0.00004	0.00014	0.00009	-3.12141
D22	-0.96003	0.00000	-0.00003	0.00009	0.00007	-0.95996
D23	1.06797	0.00000	-0.00002	0.00007	0.00005	1.06801
D24	-0.93495	0.00000	0.00000	0.00001	0.00001	-0.93494
D25	2.21511	0.00000	0.00000	-0.00004	-0.00004	2.21507
D26	-3.12595	0.00000	-0.00001	0.00008	0.00006	-3.12589
D27	0.02411	0.00000	-0.00002	0.00003	0.00001	0.02412
D28	1.03165	0.00000	0.00000	0.00001	0.00001	1.03166
D29	-2.10147	0.00000	-0.00001	-0.00004	-0.00004	-2.10151
D30	-0.93050	0.00000	0.00003	0.00002	0.00006	-0.93044
D31	1.04480	0.00000	0.00002	0.00004	0.00006	1.04486
D32	-3.11691	0.00000	0.00001	0.00003	0.00004	-3.11687
D33	2.21137	0.00000	0.00002	0.00000	0.00003	2.21140
D34	-2.09652	0.00000	0.00001	0.00002	0.00003	-2.09649
D35	0.02495	0.00000	0.00000	0.00001	0.00001	0.02496
D36	0.00389	0.00000	0.00001	0.00003	0.00004	0.00393
D37	3.13763	0.00000	0.00001	-0.00001	0.00000	3.13763
D38	-3.13799	0.00000	0.00002	0.00005	0.00007	-3.13792
D39	-0.00425	0.00000	0.00002	0.00001	0.00003	-0.00422

This journal is © The Royal Society of Chemistry 2014

D40	-0.04001	0.00000	0.00003	-0.00013	-0.00010	-0.04011
D41	-2.15438	0.00000	0.00004	-0.00018	-0.00013	-2.15451
D42	2.08392	0.00000	0.00004	-0.00016	-0.00012	2.08380
D43	2.08348	0.00000	0.00004	-0.00020	-0.00016	2.08332
D44	-0.03089	0.00000	0.00005	-0.00024	-0.00019	-0.03108
D45	-2.07577	0.00000	0.00005	-0.00023	-0.00018	-2.07595
D46	-2.15352	0.00000	0.00003	-0.00013	-0.00010	-2.15362
D47	2.01530	0.00000	0.00004	-0.00018	-0.00014	2.01516
D48	-0.02959	0.00000	0.00004	-0.00017	-0.00013	-0.02971
D49	-2.06476	0.00001	-0.00006	0.00037	0.00031	-2.06445
D50	1.07821	0.00000	-0.00009	0.00040	0.00032	1.07853
D51	2.11813	0.00000	-0.00004	0.00035	0.00031	2.11844
D52	-1.02209	0.00000	-0.00006	0.00038	0.00031	-1.02177
D53	0.02037	0.00000	-0.00004	0.00032	0.00027	0.02064
D54	-3.11985	0.00000	-0.00007	0.00035	0.00028	-3.11957
D55	-0.01208	0.00000	0.00001	-0.00005	-0.00004	-0.01212
D56	-3.13496	0.00000	0.00000	-0.00005	-0.00004	-3.13501
D57	3.12162	0.00000	0.00001	0.00000	0.00001	3.12162
D58	-0.00127	0.00000	0.00001	0.00000	0.00001	-0.00126
D59	0.00140	0.00000	-0.00001	0.00005	0.00005	0.00145
D60	3.14087	0.00000	0.00002	0.00008	0.00010	3.14097
D61	-3.13126	0.00000	-0.00001	0.00000	-0.00001	-3.13127
D62	0.00820	0.00000	0.00001	0.00003	0.00004	0.00825
D63	0.94165	0.00000	-0.00002	0.00006	0.00004	0.94168
D64	-1.01951	0.00000	0.00000	0.00004	0.00003	-1.01947
D65	3.11294	0.00000	0.00000	0.00001	0.00001	3.11296

D66	-2.21993	0.00000	-0.00002	0.00005	0.00004	-2.21989
D67	2.10211	0.00000	0.00000	0.00003	0.00003	2.10214
D68	-0.04863	0.00000	0.00001	0.00000	0.00001	-0.04862
D69	3.13136	0.00000	0.00001	-0.00002	-0.00001	3.13136
D70	-0.00686	0.00000	-0.00002	-0.00003	-0.00005	-0.00691
D71	0.01123	0.00000	0.00001	-0.00001	-0.00001	0.01122
D72	-3.12699	0.00000	-0.00003	-0.00002	-0.00005	-3.12704
D73	-0.97473	0.00000	-0.00003	0.00007	0.00004	-0.97469
D74	1.18575	0.00000	-0.00002	0.00007	0.00005	1.18580
D75	-2.99928	0.00000	-0.00004	0.00010	0.00006	-2.99922
D76	1.01491	0.00000	-0.00002	0.00006	0.00004	1.01494
D77	-3.10780	0.00000	-0.00002	0.00007	0.00005	-3.10775
D78	-1.00964	0.00000	-0.00004	0.00009	0.00005	-1.00959
D79	-3.09912	0.00000	-0.00003	0.00011	0.00008	-3.09903
D80	-0.93863	0.00000	-0.00002	0.00011	0.00009	-0.93854
D81	1.15952	0.00000	-0.00004	0.00014	0.00010	1.15962
D82	0.03067	0.00000	-0.00003	-0.00003	-0.00005	0.03061
D83	-3.12876	0.00000	0.00010	-0.00011	-0.00001	-3.12877
D84	2.11034	0.00000	-0.00002	-0.00003	-0.00005	2.11029
D85	-1.04909	0.00000	0.00010	-0.00011	0.00000	-1.04909
D86	-2.07125	0.00000	-0.00004	0.00001	-0.00003	-2.07128
D87	1.05251	0.00000	0.00008	-0.00006	0.00002	1.05253
D88	-0.00701	0.00000	-0.00002	-0.00003	-0.00005	-0.00706
D89	3.13820	0.00000	0.00000	-0.00003	-0.00003	3.13817
D90	3.13245	0.00000	0.00000	0.00000	0.00000	3.13245
D91	-0.00553	0.00000	0.00002	0.00000	0.00002	-0.00551

```
   D92       -3.13828   0.00000   0.00001   0.00002   0.00003  -
3.13825
   D93        0.00807   0.00000   0.00001   0.00003   0.00004
0.00811
   D94        0.00668   0.00000  -0.00002   0.00001  -0.00001
0.00667
   D95       -3.13016   0.00000  -0.00002   0.00001   0.00000  -
3.13016
   D96       -0.00118   0.00000   0.00001   0.00000   0.00001  -
0.00117
   D97        3.13679   0.00000  -0.00001   0.00000  -0.00001
3.13678
   D98       -3.13799   0.00000   0.00001   0.00001   0.00002  -
3.13797
   D99       -0.00002   0.00000  -0.00001   0.00001   0.00000  -
0.00003
   D100      -3.13352   0.00000  -0.00001   0.00000  -0.00001  -
3.13353
   D101       0.00550   0.00000   0.00000   0.00000   0.00000
0.00551
   D102       0.00219   0.00000  -0.00001   0.00002   0.00001
0.00220
   D103       3.14122   0.00000   0.00000   0.00002   0.00002
3.14124
   D104      -3.13889   0.00000  -0.00001   0.00001   0.00001  -
3.13888
   D105      -0.00020   0.00000  -0.00001   0.00002   0.00001  -
0.00019
   D106       0.00013   0.00000   0.00001   0.00001   0.00002
0.00015
   D107       3.13882   0.00000   0.00001   0.00002   0.00002
3.13884
   D108      -0.00448   0.00000   0.00000  -0.00004  -0.00004  -
0.00452
   D109      -3.13824   0.00000   0.00000   0.00000   0.00001  -
3.13823
   D110       3.13422   0.00000   0.00000  -0.00003  -0.00003
3.13419
   D111       0.00046   0.00000   0.00000   0.00001   0.00001
0.00048
   D112      -0.00121   0.00000   0.00003  -0.00035  -0.00033  -
0.00153
   D113       3.13912   0.00000   0.00005  -0.00038  -0.00033
3.13879
   D114      -0.01920   0.00000   0.00000   0.00024   0.00024  -
0.01896
   D115       3.13869   0.00000  -0.00011   0.00031   0.00019
3.13889
         Item               Value     Threshold  Converged?
 Maximum Force            0.000059     0.000450     YES
 RMS     Force            0.000008     0.000300     YES
 Maximum Displacement     0.001074     0.001800     YES
```

This journal is © The Royal Society of Chemistry 2014

```
 RMS     Displacement     0.000134     0.001200     YES
 Predicted change in Energy=-3.343085D-08
 Optimization completed.
    -- Stationary point found.
                           ----------------------------
                           !   Optimized Parameters   !
                           ! (Angstroms and Degrees)  !
 --------------------------                            ---------------
-----------
 ! Name  Definition              Value          Derivative Info.
!
 ---------------------------------------------------------------------
-----------
 ! R1    R(1,2)                  1.5173         -DE/DX =    0.0
!
 ! R2    R(1,4)                  1.4049         -DE/DX =    0.0
!
 ! R3    R(1,20)                 1.3926         -DE/DX =    0.0
!
 ! R4    R(2,3)                  1.0925         -DE/DX =    0.0
!
 ! R5    R(2,5)                  1.5699         -DE/DX =    0.0
!
 ! R6    R(2,7)                  1.5185         -DE/DX =    0.0
!
 ! R7    R(4,9)                  1.5402         -DE/DX =    0.0
!
 ! R8    R(4,26)                 1.3922         -DE/DX =    0.0
!
 ! R9    R(5,6)                  1.0942         -DE/DX =    0.0
!
 ! R10   R(5,10)                 1.5421         -DE/DX =    0.0
!
 ! R11   R(5,28)                 1.5206         -DE/DX =    0.0
!
 ! R12   R(7,8)                  1.4055         -DE/DX =    0.0
!
 ! R13   R(7,12)                 1.3935         -DE/DX =    0.0
!
 ! R14   R(8,9)                  1.5351         -DE/DX =    0.0
!
 ! R15   R(8,14)                 1.3924         -DE/DX =    0.0
!
 ! R16   R(9,10)                 1.5882         -DE/DX =    0.0
!
 ! R17   R(9,33)                 1.4646         -DE/DX =    0.0
!
 ! R18   R(10,11)                1.094          -DE/DX =    0.0
!
 ! R19   R(10,29)                1.528          -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! R20   R(12,13)                1.0873         -DE/DX =    0.0
!
 ! R21   R(12,18)                1.4003         -DE/DX =    0.0
!
 ! R22   R(14,15)                1.0865         -DE/DX =    0.0
!
 ! R23   R(14,16)                1.4005         -DE/DX =    0.0
!
 ! R24   R(16,17)                1.0864         -DE/DX =    0.0
!
 ! R25   R(16,18)                1.3969         -DE/DX =    0.0
!
 ! R26   R(18,19)                1.0866         -DE/DX =    0.0
!
 ! R27   R(20,21)                1.0877         -DE/DX =    0.0
!
 ! R28   R(20,22)                1.4012         -DE/DX =    0.0
!
 ! R29   R(22,23)                1.0867         -DE/DX =    0.0
!
 ! R30   R(22,24)                1.3963         -DE/DX =    0.0
!
 ! R31   R(24,25)                1.0865         -DE/DX =    0.0
!
 ! R32   R(24,26)                1.4015         -DE/DX =    0.0
!
 ! R33   R(26,27)                1.0865         -DE/DX =    0.0
!
 ! R34   R(28,30)                1.3876         -DE/DX =    0.0
!
 ! R35   R(28,32)                1.1983         -DE/DX =    0.0
!
 ! R36   R(29,30)                1.3918         -DE/DX =    0.0001
!
 ! R37   R(29,31)                1.1958         -DE/DX =    0.0
!
 ! R38   R(33,34)                1.1605         -DE/DX =    0.0
!
 ! A1    A(2,1,4)              113.7076         -DE/DX =    0.0
!
 ! A2    A(2,1,20)             126.2125         -DE/DX =    0.0
!
 ! A3    A(4,1,20)             120.0749         -DE/DX =    0.0
!
 ! A4    A(1,2,3)              113.0829         -DE/DX =    0.0
!
 ! A5    A(1,2,5)              104.9416         -DE/DX =    0.0
!
 ! A6    A(1,2,7)              107.902          -DE/DX =    0.0
!
 ! A7    A(3,2,5)              110.3852         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A8    A(3,2,7)              112.6464         -DE/DX =    0.0
!
 ! A9    A(5,2,7)              107.448          -DE/DX =    0.0
!
 ! A10   A(1,4,9)              112.9514         -DE/DX =    0.0
!
 ! A11   A(1,4,26)             120.6527         -DE/DX =    0.0
!
 ! A12   A(9,4,26)             126.3959         -DE/DX =    0.0
!
 ! A13   A(2,5,6)              108.8696         -DE/DX =    0.0
!
 ! A14   A(2,5,10)             110.0928         -DE/DX =    0.0
!
 ! A15   A(2,5,28)             112.5271         -DE/DX =    0.0
!
 ! A16   A(6,5,10)             112.5702         -DE/DX =    0.0
!
 ! A17   A(6,5,28)             108.2161         -DE/DX =    0.0
!
 ! A18   A(10,5,28)            104.5556         -DE/DX =    0.0
!
 ! A19   A(2,7,8)              113.9839         -DE/DX =    0.0
!
 ! A20   A(2,7,12)             126.0632         -DE/DX =    0.0
!
 ! A21   A(8,7,12)             119.9511         -DE/DX =    0.0
!
 ! A22   A(7,8,9)              112.7156         -DE/DX =    0.0
!
 ! A23   A(7,8,14)             120.8048         -DE/DX =    0.0
!
 ! A24   A(9,8,14)             126.4697         -DE/DX =    0.0
!
 ! A25   A(4,9,8)              107.592          -DE/DX =    0.0
!
 ! A26   A(4,9,10)             105.2185         -DE/DX =    0.0
!
 ! A27   A(4,9,33)             111.973          -DE/DX =    0.0
!
 ! A28   A(8,9,10)             106.4191         -DE/DX =    0.0
!
 ! A29   A(8,9,33)             113.4148         -DE/DX =    0.0
!
 ! A30   A(10,9,33)            111.7166         -DE/DX =    0.0
!
 ! A31   A(5,10,9)             109.6286         -DE/DX =    0.0
!
 ! A32   A(5,10,11)            112.9544         -DE/DX =    0.0
!
 ! A33   A(5,10,29)            104.2085         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A34   A(9,10,11)            108.5153         -DE/DX =    0.0
!
 ! A35   A(9,10,29)            113.4058         -DE/DX =    0.0
!
 ! A36   A(11,10,29)           108.1673         -DE/DX =    0.0
!
 ! A37   A(7,12,13)            120.1303         -DE/DX =    0.0
!
 ! A38   A(7,12,18)            119.4422         -DE/DX =    0.0
!
 ! A39   A(13,12,18)           120.4274         -DE/DX =    0.0
!
 ! A40   A(8,14,15)            120.5234         -DE/DX =    0.0
!
 ! A41   A(8,14,16)            118.9894         -DE/DX =    0.0
!
 ! A42   A(15,14,16)           120.4869         -DE/DX =    0.0
!
 ! A43   A(14,16,17)           119.5213         -DE/DX =    0.0
!
 ! A44   A(14,16,18)           120.4608         -DE/DX =    0.0
!
 ! A45   A(17,16,18)           120.0173         -DE/DX =    0.0
!
 ! A46   A(12,18,16)           120.3488         -DE/DX =    0.0
!
 ! A47   A(12,18,19)           119.6951         -DE/DX =    0.0
!
 ! A48   A(16,18,19)           119.9558         -DE/DX =    0.0
!
 ! A49   A(1,20,21)            120.1628         -DE/DX =    0.0
!
 ! A50   A(1,20,22)            119.4772         -DE/DX =    0.0
!
 ! A51   A(21,20,22)           120.3591         -DE/DX =    0.0
!
 ! A52   A(20,22,23)           119.7461         -DE/DX =    0.0
!
 ! A53   A(20,22,24)           120.249          -DE/DX =    0.0
!
 ! A54   A(23,22,24)           120.0048         -DE/DX =    0.0
!
 ! A55   A(22,24,25)           120.0377         -DE/DX =    0.0
!
 ! A56   A(22,24,26)           120.4546         -DE/DX =    0.0
!
 ! A57   A(25,24,26)           119.5075         -DE/DX =    0.0
!
 ! A58   A(4,26,24)            119.0903         -DE/DX =    0.0
!
 ! A59   A(4,26,27)            120.5669         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! A60   A(24,26,27)           120.3413         -DE/DX =    0.0
!
 ! A61   A(5,28,30)            109.8869         -DE/DX =    0.0
!
 ! A62   A(5,28,32)            128.3634         -DE/DX =    0.0
!
 ! A63   A(30,28,32)           121.7496         -DE/DX =    0.0
!
 ! A64   A(10,29,30)           109.6408         -DE/DX =    0.0
!
 ! A65   A(10,29,31)           128.8255         -DE/DX =    0.0
!
 ! A66   A(30,29,31)           121.5258         -DE/DX =    0.0
!
 ! A67   A(28,30,29)           111.6754         -DE/DX =    0.0
!
 ! A68   L(9,33,34,4,-1)       177.2989         -DE/DX =    0.0
!
 ! A69   L(9,33,34,4,-2)       178.6278         -DE/DX =    0.0
!
 ! D1    D(4,1,2,3)            179.4747         -DE/DX =    0.0
!
 ! D2    D(4,1,2,5)            -60.1525         -DE/DX =    0.0
!
 ! D3    D(4,1,2,7)             54.1985         -DE/DX =    0.0
!
 ! D4    D(20,1,2,3)            -1.3353         -DE/DX =    0.0
!
 ! D5    D(20,1,2,5)           119.0375         -DE/DX =    0.0
!
 ! D6    D(20,1,2,7)          -126.6116         -DE/DX =    0.0
!
 ! D7    D(2,1,4,9)             -0.6607         -DE/DX =    0.0
!
 ! D8    D(2,1,4,26)           179.3247         -DE/DX =    0.0
!
 ! D9    D(20,1,4,9)          -179.9055         -DE/DX =    0.0
!
 ! D10   D(20,1,4,26)            0.0799         -DE/DX =    0.0
!
 ! D11   D(2,1,20,21)            0.8446         -DE/DX =    0.0
!
 ! D12   D(2,1,20,22)         -179.4917         -DE/DX =    0.0
!
 ! D13   D(4,1,20,21)          179.9876         -DE/DX =    0.0
!
 ! D14   D(4,1,20,22)           -0.3487         -DE/DX =    0.0
!
 ! D15   D(1,2,5,6)            -64.1809         -DE/DX =    0.0
!
 ! D16   D(1,2,5,10)            59.6627         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D17   D(1,2,5,28)          175.8583         -DE/DX =    0.0
!
 ! D18   D(3,2,5,6)            57.9637         -DE/DX =    0.0
!
 ! D19   D(3,2,5,10)         -178.1927         -DE/DX =    0.0
!
 ! D20   D(3,2,5,28)           -61.997         -DE/DX =    0.0
!
 ! D21   D(7,2,5,6)          -178.8492         -DE/DX =    0.0
!
 ! D22   D(7,2,5,10)           -55.0056         -DE/DX =    0.0
!
 ! D23   D(7,2,5,28)            61.19         -DE/DX =    0.0
!
 ! D24   D(1,2,7,8)            -53.5685         -DE/DX =    0.0
!
 ! D25   D(1,2,7,12)           126.9167         -DE/DX =    0.0
!
 ! D26   D(3,2,7,8)          -179.1037         -DE/DX =    0.0
!
 ! D27   D(3,2,7,12)             1.3815         -DE/DX =    0.0
!
 ! D28   D(5,2,7,8)             59.1093         -DE/DX =    0.0
!
 ! D29   D(5,2,7,12)         -120.4055         -DE/DX =    0.0
!
 ! D30   D(1,4,9,8)             -53.3135         -DE/DX =    0.0
!
 ! D31   D(1,4,9,10)            59.8627         -DE/DX =    0.0
!
 ! D32   D(1,4,9,33)          -178.5859         -DE/DX =    0.0
!
 ! D33   D(26,4,9,8)           126.7022         -DE/DX =    0.0
!
 ! D34   D(26,4,9,10)         -120.1217         -DE/DX =    0.0
!
 ! D35   D(26,4,9,33)            1.4297         -DE/DX =    0.0
!
 ! D36   D(1,4,26,24)            0.223         -DE/DX =    0.0
!
 ! D37   D(1,4,26,27)          179.773         -DE/DX =    0.0
!
 ! D38   D(9,4,26,24)         -179.7938         -DE/DX =    0.0
!
 ! D39   D(9,4,26,27)           -0.2437         -DE/DX =    0.0
!
 ! D40   D(2,5,10,9)            -2.2926         -DE/DX =    0.0
!
 ! D41   D(2,5,10,11)         -123.4369         -DE/DX =    0.0
!
 ! D42   D(2,5,10,29)          119.3998         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D43   D(6,5,10,9)           119.3747         -DE/DX =    0.0
!
 ! D44   D(6,5,10,11)           -1.7696         -DE/DX =    0.0
!
 ! D45   D(6,5,10,29)         -118.9329         -DE/DX =    0.0
!
 ! D46   D(28,5,10,9)         -123.3877         -DE/DX =    0.0
!
 ! D47   D(28,5,10,11)         115.468          -DE/DX =    0.0
!
 ! D48   D(28,5,10,29)          -1.6953         -DE/DX =    0.0
!
 ! D49   D(2,5,28,30)         -118.3018         -DE/DX =    0.0
!
 ! D50   D(2,5,28,32)           61.7769         -DE/DX =    0.0
!
 ! D51   D(6,5,28,30)          121.3601         -DE/DX =    0.0
!
 ! D52   D(6,5,28,32)          -58.5612         -DE/DX =    0.0
!
 ! D53   D(10,5,28,30)           1.167          -DE/DX =    0.0
!
 ! D54   D(10,5,28,32)        -178.7542         -DE/DX =    0.0
!
 ! D55   D(2,7,8,9)              -0.692          -DE/DX =    0.0
!
 ! D56   D(2,7,8,14)           -179.6202         -DE/DX =    0.0
!
 ! D57   D(12,7,8,9)            178.8554         -DE/DX =    0.0
!
 ! D58   D(12,7,8,14)            -0.0728         -DE/DX =    0.0
!
 ! D59   D(2,7,12,13)             0.0803         -DE/DX =    0.0
!
 ! D60   D(2,7,12,18)           179.9584         -DE/DX =    0.0
!
 ! D61   D(8,7,12,13)          -179.408          -DE/DX =    0.0
!
 ! D62   D(8,7,12,18)             0.4701         -DE/DX =    0.0
!
 ! D63   D(7,8,9,4)              53.9523         -DE/DX =    0.0
!
 ! D64   D(7,8,9,10)            -58.4135         -DE/DX =    0.0
!
 ! D65   D(7,8,9,33)            178.3585         -DE/DX =    0.0
!
 ! D66   D(14,8,9,4)           -127.1924         -DE/DX =    0.0
!
 ! D67   D(14,8,9,10)           120.4418         -DE/DX =    0.0
!
 ! D68   D(14,8,9,33)            -2.7862         -DE/DX =    0.0
!
```

This journal is © The Royal Society of Chemistry 2014

```
 ! D69   D(7,8,14,15)          179.414          -DE/DX =    0.0
!
 ! D70   D(7,8,14,16)           -0.3929         -DE/DX =    0.0
!
 ! D71   D(9,8,14,15)            0.6434         -DE/DX =    0.0
!
 ! D72   D(9,8,14,16)         -179.1635         -DE/DX =    0.0
!
 ! D73   D(4,9,10,5)           -55.848          -DE/DX =    0.0
!
 ! D74   D(4,9,10,11)           67.9385         -DE/DX =    0.0
!
 ! D75   D(4,9,10,29)         -171.8459         -DE/DX =    0.0
!
 ! D76   D(8,9,10,5)            58.1498         -DE/DX =    0.0
!
 ! D77   D(8,9,10,11)         -178.0637         -DE/DX =    0.0
!
 ! D78   D(8,9,10,29)           -57.8481        -DE/DX =    0.0
!
 ! D79   D(33,9,10,5)         -177.5662         -DE/DX =    0.0
!
 ! D80   D(33,9,10,11)          -53.7797        -DE/DX =    0.0
!
 ! D81   D(33,9,10,29)           66.4359        -DE/DX =    0.0
!
 ! D82   D(5,10,29,30)            1.7572        -DE/DX =    0.0
!
 ! D83   D(5,10,29,31)         -179.2646         -DE/DX =    0.0
!
 ! D84   D(9,10,29,30)          120.9133         -DE/DX =    0.0
!
 ! D85   D(9,10,29,31)          -60.1085         -DE/DX =    0.0
!
 ! D86   D(11,10,29,30)        -118.6737         -DE/DX =    0.0
!
 ! D87   D(11,10,29,31)          60.3045         -DE/DX =    0.0
!
 ! D88   D(7,12,18,16)           -0.4016         -DE/DX =    0.0
!
 ! D89   D(7,12,18,19)          179.8054         -DE/DX =    0.0
!
 ! D90   D(13,12,18,16)         179.4762         -DE/DX =    0.0
!
 ! D91   D(13,12,18,19)          -0.3168         -DE/DX =    0.0
!
 ! D92   D(8,14,16,17)         -179.8101         -DE/DX =    0.0
!
 ! D93   D(8,14,16,18)            0.4622         -DE/DX =    0.0
!
 ! D94   D(15,14,16,17)           0.3829         -DE/DX =    0.0
!
```

```
 ! D95   D(15,14,16,18)       -179.3448         -DE/DX =    0.0
!
 ! D96   D(14,16,18,12)         -0.0674         -DE/DX =    0.0
!
 ! D97   D(14,16,18,19)        179.725          -DE/DX =    0.0
!
 ! D98   D(17,16,18,12)       -179.7938         -DE/DX =    0.0
!
 ! D99   D(17,16,18,19)         -0.0013         -DE/DX =    0.0
!
 ! D100  D(1,20,22,23)         -179.5376         -DE/DX =    0.0
!
 ! D101  D(1,20,22,24)           0.3154         -DE/DX =    0.0
!
 ! D102  D(21,20,22,23)          0.1254         -DE/DX =    0.0
!
 ! D103  D(21,20,22,24)        179.9784         -DE/DX =    0.0
!
 ! D104  D(20,22,24,25)       -179.8451         -DE/DX =    0.0
!
 ! D105  D(20,22,24,26)         -0.0117         -DE/DX =    0.0
!
 ! D106  D(23,22,24,25)          0.0076         -DE/DX =    0.0
!
 ! D107  D(23,22,24,26)        179.841          -DE/DX =    0.0
!
 ! D108  D(22,24,26,4)          -0.2567         -DE/DX =    0.0
!
 ! D109  D(22,24,26,27)       -179.8077         -DE/DX =    0.0
!
 ! D110  D(25,24,26,4)         179.5776         -DE/DX =    0.0
!
 ! D111  D(25,24,26,27)          0.0265         -DE/DX =    0.0
!
 ! D112  D(5,28,30,29)          -0.0691         -DE/DX =    0.0
!
 ! D113  D(32,28,30,29)        179.8583         -DE/DX =    0.0
!
 ! D114  D(10,29,30,28)         -1.0999         -DE/DX =    0.0
!
 ! D115  D(31,29,30,28)        179.8339         -DE/DX =    0.0
!
 ---------------------------------------------------------------------
-----------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGr
ad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

This journal is © The Royal Society of Chemistry 2014

1	6	0	-1.657134	-1.063444	-0.025040
2	6	0	-0.228244	-1.573561	-0.040814
3	1	0	-0.161299	-2.662083	0.024050
4	6	0	-1.758123	0.335970	-0.096116
5	6	0	0.366526	-1.069346	-1.403336
6	1	0	-0.178057	-1.544796	-2.224746
7	6	0	0.529531	-0.873745	1.073519
8	6	0	0.445541	0.528538	1.028489
9	6	0	-0.386917	1.034733	-0.157789
10	6	0	0.310029	0.470367	-1.468618
11	1	0	-0.237732	0.840633	-2.340190
12	6	0	1.270463	-1.494455	2.077293
13	1	0	1.345318	-2.578736	2.109262
14	6	0	1.094444	1.312651	1.978740
15	1	0	1.034241	2.396544	1.934055
16	6	0	1.829517	0.682983	2.990951
17	1	0	2.336681	1.286338	3.738664
18	6	0	1.917796	-0.710225	3.039944
19	1	0	2.494031	-1.190049	3.826325
20	6	0	-2.808772	-1.844084	0.034865
21	1	0	-2.732252	-2.927681	0.089724
22	6	0	-4.064309	-1.222101	0.031011
23	1	0	-4.965660	-1.826653	0.085218
24	6	0	-4.159856	0.169177	-0.039032
25	1	0	-5.135149	0.648026	-0.039254
26	6	0	-3.003494	0.958133	-0.105912
27	1	0	-3.079911	2.040731	-0.157217
28	6	0	1.842016	-1.404362	-1.554441
29	6	0	1.771429	0.893655	-1.609278
30	8	0	2.582319	-0.236056	-1.665684
31	8	0	2.228681	1.995956	-1.685355
32	8	0	2.360274	-2.484402	-1.583303
33	6	0	-0.516317	2.493040	-0.197843
34	7	0	-0.672509	3.642913	-0.210815

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.517299	0.000000			
3	H	2.189881	1.092506	0.000000		
4	C	1.404853	2.447426	3.398913	0.000000	
5	C	2.448456	1.569857	2.202917	2.863192	0.000000
6	H	2.694081	2.184698	2.511114	3.250377	1.094229
7	C	2.454450	1.518455	2.185586	2.839862	2.489909
8	C	2.839996	2.452797	3.399590	2.481522	2.910885
9	C	2.456303	2.615733	3.708156	1.540220	2.558557
10	C	2.882052	2.550686	3.501778	2.485775	1.542131
11	H	3.316644	3.333999	4.226640	2.757198	2.211524
12	C	3.629931	2.595912	2.762083	4.152890	3.621133
13	H	3.983224	2.847683	2.573898	4.794846	3.946472
14	C	4.151162	3.762754	4.603934	3.660064	4.200263

This journal is © The Royal Society of Chemistry 2014

15	H	4.801361	4.610391	5.537792	4.020553	4.857614
16	C	4.929802	4.303251	4.894417	4.745688	4.951844
17	H	5.969716	5.389093	5.968944	5.690005	5.989234
18	C	4.722184	3.852520	4.150663	4.943863	4.719974
19	H	5.664029	4.744748	4.865692	5.982900	5.647142
20	C	1.392572	2.595772	2.770984	2.423563	3.570877
21	H	2.155093	2.849690	2.585469	3.410994	3.909611
22	C	2.413049	3.852801	4.160178	2.786080	4.659720
23	H	3.397202	4.745845	4.876839	3.872740	5.587622
24	C	2.789833	4.300548	4.899843	2.408195	4.887065
25	H	3.876328	5.386387	5.974948	3.391890	5.922712
26	C	2.430226	3.757089	4.604446	1.392168	4.141378
27	H	3.417260	4.605286	5.537834	2.158024	4.806591
28	C	3.833972	2.570150	2.843724	4.256344	1.520572
29	C	4.253833	3.542023	4.364226	3.880517	2.422712
30	O	4.620525	3.511180	4.033392	4.650827	2.381793
31	O	5.216909	4.634916	5.507395	4.601721	3.597670
32	O	4.537276	3.147909	2.995578	5.208398	2.451490
33	C	3.738972	4.079815	5.172095	2.491060	3.863058
34	N	4.811839	5.238117	6.330045	3.482468	4.970621

		6	7	8	9	10
6	H	0.000000				
7	C	3.439410	0.000000			
8	C	3.907829	1.405517	0.000000		
9	C	3.312085	2.449139	1.535082	0.000000	
10	C	2.206998	2.883969	2.501458	1.588243	0.000000
11	H	2.388966	3.896305	3.451415	2.196088	1.093973
12	C	4.539635	1.393493	2.423424	3.760225	4.166106
13	H	4.708856	2.155288	3.410692	4.604054	4.813530
14	C	5.239614	2.432874	1.392438	2.614655	3.634422
15	H	5.856573	3.419070	2.157791	2.872286	3.976533
16	C	6.016381	2.791041	2.406345	3.866635	4.716121
17	H	7.064099	3.877467	3.390534	4.760634	5.647027
18	C	5.727659	2.412643	2.783526	4.310694	4.930095
19	H	6.624301	3.396653	3.870108	5.396544	5.963494
20	C	3.480815	3.628309	4.148153	3.766973	4.164621
21	H	3.713899	3.978157	4.788015	4.611137	4.819816
22	C	4.505055	4.723509	4.939478	4.318815	4.924243
23	H	5.323205	5.664088	5.976435	5.404764	5.960168
24	C	4.854871	4.931105	4.741142	3.872772	4.702585
25	H	5.844450	5.970146	5.683173	4.765428	5.632460
26	C	4.328649	4.150794	3.656126	2.618212	3.615843
27	H	5.054843	4.799682	4.015151	2.874761	3.959484
28	C	2.133009	2.985021	3.515363	3.587195	2.422593
29	C	3.182034	3.444331	2.974745	2.604838	1.527955
30	O	3.105645	3.481928	3.522640	3.564409	2.387712
31	O	4.315119	4.328242	3.563405	3.177854	2.460817
32	O	2.781624	3.606181	4.423287	4.686519	3.598238
33	C	4.530660	3.747719	2.507655	1.464584	2.527632
34	N	5.586835	4.847123	3.533446	2.624304	3.551407

		11	12	13	14	15
11	H	0.000000				

This journal is © The Royal Society of Chemistry 2014

12	C	5.219333	0.000000			
13	H	5.830587	1.087332	0.000000		
14	C	4.544298	2.814346	3.901649	0.000000	
15	H	4.723128	3.900793	4.988073	1.086482	0.000000
16	C	5.720090	2.426633	3.413303	1.400495	2.164667
17	H	6.616549	3.410247	4.310052	2.154340	2.487071
18	C	5.999775	1.400270	2.164540	2.428187	3.414041
19	H	7.043586	2.156130	2.489237	3.411147	4.309910
20	C	4.411217	4.575359	4.700989	5.383189	6.029809
21	H	5.131013	4.693217	4.563647	6.016011	6.777565
22	C	4.951783	5.720248	5.951777	6.068884	6.535394
23	H	5.945613	6.554993	6.670144	7.082761	7.566531
24	C	4.596655	6.060929	6.517141	5.743396	5.986057
25	H	5.414434	7.078267	7.551461	6.581934	6.709145
26	C	3.557420	5.389645	6.027321	4.611350	4.746977
27	H	3.779363	6.034594	6.786682	4.745276	4.628851
28	C	3.159550	3.677538	3.879250	4.519335	5.221972
29	C	2.138638	4.420955	5.105547	3.675288	3.918843
30	O	3.093041	4.161059	4.611782	4.230140	4.720725
31	O	2.801209	5.220984	6.008931	3.896022	3.832400
32	O	4.287000	3.945585	3.830674	5.357993	6.160666
33	C	2.719873	4.926352	5.874634	2.953875	2.637902
34	N	3.546271	5.950052	6.939978	3.653271	3.011129

		16	17	18	19	20
16	C	0.000000				
17	H	1.086429	0.000000			
18	C	1.396862	2.156371	0.000000		
19	H	2.155848	2.482929	1.086588	0.000000	
20	C	6.052953	7.070598	5.714594	6.551539	0.000000
21	H	6.501057	7.534374	5.936654	6.655493	1.087679
22	C	6.864967	7.810995	6.715749	7.577418	1.401161
23	H	7.804869	8.738568	7.573558	8.369476	2.157546
24	C	6.731818	7.597633	6.869592	7.814262	2.425718
25	H	7.595389	8.396925	7.814752	8.747892	3.410005
26	C	5.746674	6.588320	6.074449	7.092246	2.812499
27	H	5.988064	6.714646	6.539623	7.574653	3.899000
28	C	5.001775	5.958316	4.647144	5.424362	4.934478
29	C	4.605417	5.392050	4.920277	5.865983	5.583607
30	O	4.805787	5.620053	4.775915	5.574950	5.877200
31	O	4.873507	5.471308	5.454220	6.371786	6.563611
32	O	5.589081	6.522451	4.971710	5.563930	5.454127
33	C	4.352889	5.009173	5.164211	6.230672	4.911227
34	N	5.027188	5.496095	6.018880	7.048617	5.893311

		21	22	23	24	25
21	H	0.000000				
22	C	2.164908	0.000000			
23	H	2.490059	1.086671	0.000000		
24	C	3.412500	1.396312	2.155944	0.000000	
25	H	4.310015	2.156156	2.483598	1.086505	0.000000
26	C	3.900178	2.428476	3.411987	1.401463	2.155125
27	H	4.986678	3.413289	4.309465	2.164016	2.485467
28	C	5.093888	6.118133	7.015074	6.387093	7.428924

29	C	6.145922	6.420500	7.460547	6.178243	7.087040
30	O	6.210552	6.930276	7.909971	6.947455	7.936384
31	O	7.211377	7.273481	8.337014	6.845503	7.665021
32	O	5.378599	6.743492	7.542274	7.206826	8.269072
33	C	5.863214	5.142266	6.207780	4.324459	4.976227
34	N	6.892428	5.935583	6.959521	4.925236	5.377168

		26	27	28	29	30
26	C	0.000000				
27	H	1.086504	0.000000			
28	C	5.581987	6.168166	0.000000		
29	C	5.006412	5.192280	2.299755	0.000000	
30	O	5.921172	6.286500	1.387575	1.391751	0.000000
31	O	5.563036	5.524342	3.424736	1.195799	2.259939
32	O	6.542456	7.218460	1.198295	3.429094	2.260786
33	C	2.924114	2.603507	4.753087	3.127933	4.382244
34	N	3.557041	2.892308	5.796822	3.935346	5.268486

		31	32	33	34	
31	O	0.000000				
32	O	4.483452	0.000000			
33	C	3.161455	5.913477	0.000000		
34	N	3.647415	6.973197	1.160505	0.000000	

Stoichiometry C19H11NO3
Framework group C1[X(C19H11NO3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.657079	-1.064686	-0.013600
2	6	0	-0.227741	-1.573747	-0.007070
3	1	0	-0.160558	-2.660664	0.080496
4	6	0	-1.758476	0.332902	-0.113989
5	6	0	0.378031	-1.096836	-1.374568
6	1	0	-0.159329	-1.589388	-2.190641
7	6	0	0.520194	-0.850726	1.099066
8	6	0	0.435575	0.550275	1.024800
9	6	0	-0.387305	1.031484	-0.178438
10	6	0	0.320974	0.441178	-1.471648
11	1	0	-0.219752	0.793143	-2.355115
12	6	0	1.253159	-1.450221	2.121412
13	1	0	1.328524	-2.533560	2.176070
14	6	0	1.075952	1.354140	1.964269
15	1	0	1.015345	2.436845	1.897028
16	6	0	1.802994	0.745856	2.995183
17	1	0	2.303460	1.364752	3.734663
18	6	0	1.891863	-0.645988	3.073263
19	1	0	2.461852	-1.109198	3.874027
20	6	0	-2.808616	-1.844968	0.052578

21	1	0	-2.731777	-2.927155	0.130121
22	6	0	-4.064523	-1.224308	0.025594
23	1	0	-4.965861	-1.828433	0.084579
24	6	0	-4.160482	0.165170	-0.073551
25	1	0	-5.136083	0.643049	-0.091655
26	6	0	-3.004169	0.953629	-0.146834
27	1	0	-3.080933	2.034891	-0.220802
28	6	0	1.854972	-1.433547	-1.506512
29	6	0	1.783194	0.862815	-1.608705
30	8	0	2.595339	-0.267089	-1.635338
31	8	0	2.240273	1.963745	-1.703391
32	8	0	2.374229	-2.513490	-1.509058
33	6	0	-0.517415	2.488558	-0.249248
34	7	0	-0.674319	3.637789	-0.286928

Rotational constants (GHZ): 0.3755593 0.2679362
0.2565006

****

Population analysis using the SCF density.

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

```
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues --  -19.24750 -19.18762 -19.18759 -14.36249 -
10.36136
 Alpha  occ. eigenvalues --  -10.36051 -10.29140 -10.26596 -10.25844 -
10.25208
 Alpha  occ. eigenvalues --  -10.24984 -10.23786 -10.23526 -10.23295 -
10.23041
 Alpha  occ. eigenvalues --  -10.22456 -10.22357 -10.22222 -10.22114 -
10.22092
 Alpha  occ. eigenvalues --  -10.22060 -10.21864 -10.21767  -1.16459
-1.09931
 Alpha  occ. eigenvalues --   -1.06074  -0.94994  -0.92405  -0.88382
-0.86644
 Alpha  occ. eigenvalues --   -0.83712  -0.80905  -0.77797  -0.77244
-0.76154
 Alpha  occ. eigenvalues --   -0.71585  -0.69791  -0.66319  -0.65567
-0.63268
 Alpha  occ. eigenvalues --   -0.63185  -0.60047  -0.58546  -0.56394
-0.54877
 Alpha  occ. eigenvalues --   -0.53469  -0.51209  -0.50873  -0.49874
-0.49271
 Alpha  occ. eigenvalues --   -0.48461  -0.47748  -0.46677  -0.46483
-0.46320
 Alpha  occ. eigenvalues --   -0.46006  -0.45229  -0.44852  -0.44097
-0.42249
 Alpha  occ. eigenvalues --   -0.41104  -0.40787  -0.39031  -0.38800
-0.38646
 Alpha  occ. eigenvalues --   -0.38025  -0.37600  -0.36874  -0.36282
-0.35443
 Alpha  occ. eigenvalues --   -0.35065  -0.34727  -0.32955  -0.30304
-0.28552
 Alpha  occ. eigenvalues --   -0.28175  -0.27845  -0.26631
 Alpha virt. eigenvalues --   -0.05890  -0.05040  -0.04683  -0.04423
-0.02714
 Alpha virt. eigenvalues --   -0.02537  -0.01249  -0.00273  -0.00062
0.00562
 Alpha virt. eigenvalues --    0.00719   0.01116   0.02393   0.02555
0.03037
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.03184   0.03656   0.04571   0.04775
0.05096
 Alpha virt. eigenvalues --    0.05951   0.06028   0.06375   0.07423
0.07691
 Alpha virt. eigenvalues --    0.08042   0.08700   0.09105   0.09178
0.09426
 Alpha virt. eigenvalues --    0.09966   0.10184   0.10815   0.11010
0.11178
 Alpha virt. eigenvalues --    0.11680   0.12183   0.12514   0.12823
0.13156
 Alpha virt. eigenvalues --    0.13459   0.13848   0.14009   0.14287
0.14696
 Alpha virt. eigenvalues --    0.15027   0.15241   0.15529   0.15909
0.16255
 Alpha virt. eigenvalues --    0.16520   0.16866   0.17206   0.17766
0.17972
 Alpha virt. eigenvalues --    0.18532   0.18688   0.18832   0.19177
0.19529
 Alpha virt. eigenvalues --    0.19709   0.20207   0.20387   0.20528
0.20741
 Alpha virt. eigenvalues --    0.21196   0.21336   0.21658   0.22018
0.22402
 Alpha virt. eigenvalues --    0.22606   0.23112   0.23343   0.23664
0.24004
 Alpha virt. eigenvalues --    0.24372   0.24557   0.24663   0.24943
0.25620
 Alpha virt. eigenvalues --    0.25847   0.26180   0.26500   0.26879
0.26973
 Alpha virt. eigenvalues --    0.27329   0.27488   0.27521   0.28002
0.28432
 Alpha virt. eigenvalues --    0.28951   0.29262   0.29471   0.29773
0.30187
 Alpha virt. eigenvalues --    0.30537   0.30865   0.31053   0.31624
0.32284
 Alpha virt. eigenvalues --    0.32598   0.32836   0.33297   0.33673
0.33988
 Alpha virt. eigenvalues --    0.34530   0.34995   0.35412   0.35796
0.36420
 Alpha virt. eigenvalues --    0.36677   0.37398   0.37926   0.38299
0.39199
 Alpha virt. eigenvalues --    0.39901   0.39968   0.40630   0.41060
0.41494
 Alpha virt. eigenvalues --    0.41987   0.43272   0.43469   0.44188
0.44493
 Alpha virt. eigenvalues --    0.45499   0.46770   0.49904   0.52045
0.55491
 Alpha virt. eigenvalues --    0.56206   0.57452   0.59261   0.61155
0.62665
 Alpha virt. eigenvalues --    0.66451   0.67246   0.68092   0.68545
0.69529
 Alpha virt. eigenvalues --    0.70136   0.70578   0.71019   0.71675
0.71945
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    0.72129   0.72995   0.73814   0.74599
0.75168
 Alpha virt. eigenvalues --    0.75608   0.76148   0.76551   0.76888
0.78005
 Alpha virt. eigenvalues --    0.79307   0.79823   0.79924   0.80255
0.80667
 Alpha virt. eigenvalues --    0.81385   0.82650   0.83257   0.83940
0.84873
 Alpha virt. eigenvalues --    0.85611   0.86378   0.87281   0.88310
0.88833
 Alpha virt. eigenvalues --    0.89211   0.89764   0.90772   0.91446
0.92485
 Alpha virt. eigenvalues --    0.93738   0.93815   0.95442   0.95727
0.95977
 Alpha virt. eigenvalues --    0.97386   0.98577   0.99267   0.99985
1.01109
 Alpha virt. eigenvalues --    1.02118   1.03070   1.04203   1.04314
1.05057
 Alpha virt. eigenvalues --    1.06754   1.07776   1.08038   1.09177
1.09298
 Alpha virt. eigenvalues --    1.11995   1.12481   1.14103   1.14717
1.15954
 Alpha virt. eigenvalues --    1.17150   1.17936   1.18362   1.20774
1.21122
 Alpha virt. eigenvalues --    1.21375   1.22555   1.23616   1.24746
1.26105
 Alpha virt. eigenvalues --    1.27338   1.28354   1.29825   1.31371
1.32354
 Alpha virt. eigenvalues --    1.33998   1.34332   1.34975   1.35087
1.36427
 Alpha virt. eigenvalues --    1.37754   1.38389   1.39302   1.40200
1.41545
 Alpha virt. eigenvalues --    1.41841   1.42607   1.43198   1.43764
1.45019
 Alpha virt. eigenvalues --    1.45547   1.46118   1.47571   1.47900
1.48373
 Alpha virt. eigenvalues --    1.49306   1.51046   1.52627   1.53732
1.55363
 Alpha virt. eigenvalues --    1.57692   1.58812   1.60215   1.62722
1.63523
 Alpha virt. eigenvalues --    1.67120   1.69108   1.69338   1.69758
1.71882
 Alpha virt. eigenvalues --    1.74832   1.76280   1.77076   1.77499
1.79458
 Alpha virt. eigenvalues --    1.79954   1.80954   1.82072   1.82506
1.83292
 Alpha virt. eigenvalues --    1.84493   1.85410   1.85885   1.86668
1.87890
 Alpha virt. eigenvalues --    1.88197   1.89566   1.90333   1.91581
1.93004
 Alpha virt. eigenvalues --    1.93222   1.94922   1.96103   1.96885
1.97143
```

This journal is © The Royal Society of Chemistry 2014

```
 Alpha virt. eigenvalues --    1.97840   1.98705   1.99957   2.00722
2.02012
 Alpha virt. eigenvalues --    2.02190   2.03190   2.04517   2.05383
2.07384
 Alpha virt. eigenvalues --    2.08446   2.10924   2.11813   2.12202
2.15093
 Alpha virt. eigenvalues --    2.16900   2.17426   2.18318   2.19870
2.20672
 Alpha virt. eigenvalues --    2.23426   2.24214   2.25218   2.25960
2.27529
 Alpha virt. eigenvalues --    2.28169   2.29339   2.30600   2.31362
2.34558
 Alpha virt. eigenvalues --    2.35412   2.37106   2.38956   2.41186
2.43089
 Alpha virt. eigenvalues --    2.46022   2.49074   2.49683   2.51849
2.53694
 Alpha virt. eigenvalues --    2.56679   2.58564   2.59423   2.62002
2.63072
 Alpha virt. eigenvalues --    2.64620   2.67545   2.68081   2.68897
2.69104
 Alpha virt. eigenvalues --    2.71481   2.72990   2.74766   2.75013
2.77205
 Alpha virt. eigenvalues --    2.78841   2.79953   2.80156   2.82690
2.83760
 Alpha virt. eigenvalues --    2.84156   2.85539   2.90044   2.93763
2.94748
 Alpha virt. eigenvalues --    2.95962   3.03784   3.05565   3.09728
3.12518
 Alpha virt. eigenvalues --    3.15329   3.22508   3.22918   3.26866
3.33239
 Alpha virt. eigenvalues --    3.34426   3.40092   3.45262   4.23059
4.25539
 Alpha virt. eigenvalues --    4.26534   4.30545   4.32714   4.34382
4.35473
 Alpha virt. eigenvalues --    4.38340   4.42044   4.43668   4.47694
4.47986
 Alpha virt. eigenvalues --    4.49376   4.51444   4.56955   4.61939
4.66966
 Alpha virt. eigenvalues --    4.73761   4.75659   4.81494   4.89149
5.15760
 Alpha virt. eigenvalues --    5.47067
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C   14.936420  -3.719735  -0.036460   1.334903  -0.076478
0.024330
     2  C   -3.719735  22.054004   0.225340  -6.951613  -2.179825  -
0.031044
     3  H   -0.036460   0.225340   0.524379   0.004554   0.003053  -
0.002835
     4  C    1.334903  -6.951613   0.004554  27.275431   1.648220
0.020313
```

This journal is © The Royal Society of Chemistry 2014

```
     5  C   -0.076478  -2.179825   0.003053   1.648220  11.307762
0.321258
     6  H    0.024330  -0.031044  -0.002835   0.020313   0.321258
0.474496
     7  C   -0.176776  -3.870966  -0.067054   0.423547   0.493327
0.021281
     8  C    3.912488 -10.313923   0.016493   0.529622   1.419114
0.008335
     9  C   -2.168936   5.885869  -0.012340  -2.929426  -2.237717  -
0.007317
    10  C    1.186099   0.079446   0.030150  -1.474276  -2.952442  -
0.009565
    11  H   -0.045745  -0.005873  -0.000113   0.086208  -0.024316  -
0.004226
    12  C   -0.395242   2.121591   0.039795  -0.926721   0.122597
0.009551
    13  H   -0.015166  -0.041697   0.003239  -0.000941  -0.008850  -
0.000005
    14  C   -2.047284   2.524796   0.001481   1.015088  -0.007622
0.001573
    15  H   -0.002389   0.006027   0.000002   0.001757   0.001573
0.000000
    16  C   -0.062522  -0.179938   0.001655  -0.011568  -0.024803  -
0.000013
    17  H    0.002261   0.002356   0.000000  -0.003650   0.000932
0.000000
    18  C   -0.308140   0.289995   0.007850  -0.031364  -0.044182
0.001390
    19  H   -0.002600  -0.016139  -0.000004   0.001744  -0.000449
0.000000
    20  C   -0.865943   0.042175   0.033274  -3.624827   0.438049  -
0.031036
    21  H   -0.020902  -0.080964   0.003335   0.086955   0.011825  -
0.000055
    22  C   -1.173660  -0.876278   0.004661  -0.749609   0.030332  -
0.005391
    23  H    0.014202  -0.013393  -0.000004   0.023140  -0.001443
0.000001
    24  C    0.038506   0.611621  -0.001745   1.902394  -0.101430
0.004834
    25  H    0.008410   0.002886   0.000000   0.024285   0.000716
0.000000
    26  C    1.076222  -0.473888   0.012113 -11.075114  -0.226071  -
0.004609
    27  H    0.031295  -0.005280   0.000002  -0.105548  -0.001028
0.000000
    28  C   -0.631759   0.733013  -0.018533  -0.462526  -1.162527  -
0.073703
    29  C   -0.382950   0.757167  -0.000687  -0.373705   0.472636
0.010374
    30  O    0.003876   0.121178  -0.000407  -0.015610  -0.349572
0.005176
```

This journal is © The Royal Society of Chemistry 2014

31	O	0.024122	-0.065776	0.000070	0.020843	-0.029622	-0.000619
32	O	0.022085	-0.117870	0.004768	0.016659	-0.004389	-0.002207
33	C	-4.025851	-1.175127	0.008266	0.203856	-0.467586	0.013076
34	N	0.088373	0.059525	-0.000025	-0.098836	0.023111	-0.000151

		7	8	9	10	11	12
1	C	-0.176776	3.912488	-2.168936	1.186099	-0.045745	-0.395242
2	C	-3.870966	-10.313923	5.885869	0.079446	-0.005873	2.121591
3	H	-0.067054	0.016493	-0.012340	0.030150	-0.000113	0.039795
4	C	0.423547	0.529622	-2.929426	-1.474276	0.086208	-0.926721
5	C	0.493327	1.419114	-2.237717	-2.952442	-0.024316	0.122597
6	H	0.021281	0.008335	-0.007317	-0.009565	-0.004226	0.009551
7	C	16.328858	3.224809	-2.807027	0.203565	0.004369	-3.940450
8	C	3.224809	44.207334	-5.100622	-1.946288	0.001420	-6.041464
9	C	-2.807027	-5.100622	19.616925	0.560033	0.011552	0.382151
10	C	0.203565	-1.946288	0.560033	11.932184	0.325609	-0.122965
11	H	0.004369	0.001420	0.011552	0.325609	0.460010	-0.002621
12	C	-3.940450	-6.041464	0.382151	-0.122965	-0.002621	10.115505
13	H	-0.073380	0.059711	0.023687	-0.000968	0.000000	0.287837
14	C	-1.258687	-20.471017	1.031064	0.153008	0.023544	3.911253
15	H	0.038252	-0.150552	-0.032618	-0.017696	-0.000005	-0.007162
16	C	0.749359	0.419075	-0.256734	0.145495	0.000665	-1.285948
17	H	0.012840	0.038244	-0.013328	-0.000240	0.000000	0.015765
18	C	-1.551344	-1.764442	0.224688	-0.018807	0.000215	1.247070
19	H	0.022517	0.036261	0.003133	0.000805	0.000000	-0.011287
20	C	1.218948	0.339229	-1.709972	-0.118037	-0.013894	-0.400673
21	H	0.007466	0.008917	0.003613	-0.002334	0.000000	0.000087

This journal is © The Royal Society of Chemistry 2014

22	C	0.113178	0.467821	-0.438412	0.025727	-0.004694	-0.200664
23	H	-0.003030	0.000502	0.004424	0.001169	0.000000	0.000519
24	C	-0.093394	-1.179245	0.116752	0.358843	0.007386	0.163016
25	H	0.000747	-0.004429	-0.012392	-0.000360	0.000001	-0.000197
26	C	0.487094	3.316200	-0.504420	0.079001	-0.050291	-0.430130
27	H	0.001969	0.021271	-0.041983	-0.001109	-0.000060	0.001009
28	C	-0.716648	-0.953355	1.029267	0.330391	0.024542	0.333605
29	C	-0.195473	-0.801314	-0.028397	-0.893692	-0.076758	0.231079
30	O	-0.099533	-0.156964	0.075220	-0.181950	0.004787	0.018292
31	O	-0.012435	0.192631	-0.022244	-0.141103	-0.000785	-0.011009
32	O	0.125529	0.073584	-0.052777	-0.061644	-0.000652	-0.083264
33	C	-2.376059	-3.330028	-4.978461	-1.438930	0.007365	0.539649
34	N	0.112415	-0.175186	0.133196	-0.027000	0.001346	0.011776

		13	14	15	16	17	18
1	C	-0.015166	-2.047284	-0.002389	-0.062522	0.002261	-0.308140
2	C	-0.041697	2.524796	0.006027	-0.179938	0.002356	0.289995
3	H	0.003239	0.001481	0.000002	0.001655	0.000000	0.007850
4	C	-0.000941	1.015088	0.001757	-0.011568	-0.003650	-0.031364
5	C	-0.008850	-0.007622	0.001573	-0.024803	0.000932	-0.044182
6	H	-0.000005	0.001573	0.000000	-0.000013	0.000000	0.001390
7	C	-0.073380	-1.258687	0.038252	0.749359	0.012840	-1.551344
8	C	0.059711	-20.471017	-0.150552	0.419075	0.038244	-1.764442
9	C	0.023687	1.031064	-0.032618	-0.256734	-0.013328	0.224688
10	C	-0.000968	0.153008	-0.017696	0.145495	-0.000240	-0.018807
11	H	0.000000	0.023544	-0.000005	0.000665	0.000000	0.000215
12	C	0.287837	3.911253	-0.007162	-1.285948	0.015765	1.247070

This journal is © The Royal Society of Chemistry 2014

13	H	0.529829	-0.014246	0.000018	0.005297	-0.000157	0.047970
14	C	-0.014246	21.746841	0.352259	-1.839512	-0.019516	0.647868
15	H	0.000018	0.352259	0.502750	0.061838	-0.003883	0.014341
16	C	0.005297	-1.839512	0.061838	8.045717	0.323893	0.681431
17	H	-0.000157	-0.019516	-0.003883	0.323893	0.518140	-0.056723
18	C	0.047970	0.647868	0.014341	0.681431	-0.056723	6.626380
19	H	-0.004186	-0.001752	-0.000149	-0.041219	-0.004170	0.305894
20	C	-0.006470	-0.634697	0.000752	-0.019714	-0.000069	-0.089265
21	H	0.000000	0.000327	0.000000	-0.000178	0.000000	0.000533
22	C	-0.000735	-0.283259	-0.000084	-0.010454	0.000029	-0.039427
23	H	0.000000	-0.000109	0.000000	-0.000016	0.000000	0.000007
24	C	-0.000037	0.542033	-0.001021	-0.015526	-0.000024	0.037940
25	H	0.000000	0.000714	0.000000	0.000005	0.000000	0.000010
26	C	0.000177	-2.383206	-0.006707	-0.003664	0.000738	-0.108031
27	H	0.000000	-0.006519	0.000001	-0.000724	0.000000	-0.000024
28	C	0.015128	0.638549	-0.000446	-0.030794	-0.001163	0.043475
29	C	-0.000978	0.211640	0.014474	-0.034999	0.001451	0.042679
30	O	-0.000115	0.036676	-0.000112	-0.015567	-0.000006	0.009731
31	O	0.000000	-0.127331	-0.000363	-0.014113	-0.000040	-0.005567
32	O	-0.000334	-0.034214	-0.000001	0.001571	0.000003	-0.015223
33	C	0.004116	2.491391	0.010405	-0.166509	-0.005690	0.051091
34	N	-0.000002	0.053761	0.005572	0.018492	0.000088	0.003749

		19	20	21	22	23	24
1	C	-0.002600	-0.865943	-0.020902	-1.173660	0.014202	0.038506
2	C	-0.016139	0.042175	-0.080964	-0.876278	-0.013393	0.611621
3	H	-0.000004	0.033274	0.003335	0.004661	-0.000004	-0.001745

This journal is © The Royal Society of Chemistry 2014

4	C	0.001744	-3.624827	0.086955	-0.749609	0.023140	1.902394
5	C	-0.000449	0.438049	0.011825	0.030332	-0.001443	-0.101430
6	H	0.000000	-0.031036	-0.000055	-0.005391	0.000001	0.004834
7	C	0.022517	1.218948	0.007466	0.113178	-0.003030	-0.093394
8	C	0.036261	0.339229	0.008917	0.467821	0.000502	-1.179245
9	C	0.003133	-1.709972	0.003613	-0.438412	0.004424	0.116752
10	C	0.000805	-0.118037	-0.002334	0.025727	0.001169	0.358843
11	H	0.000000	-0.013894	0.000000	-0.004694	0.000000	0.007386
12	C	-0.011287	-0.400673	0.000087	-0.200664	0.000519	0.163016
13	H	-0.004186	-0.006470	0.000000	-0.000735	0.000000	-0.000037
14	C	-0.001752	-0.634697	0.000327	-0.283259	-0.000109	0.542033
15	H	-0.000149	0.000752	0.000000	-0.000084	0.000000	-0.001021
16	C	-0.041219	-0.019714	-0.000178	-0.010454	-0.000016	-0.015526
17	H	-0.004170	-0.000069	0.000000	0.000029	0.000000	-0.000024
18	C	0.305894	-0.089265	0.000533	-0.039427	0.000007	0.037940
19	H	0.521486	0.000416	0.000000	0.000004	0.000000	-0.000006
20	C	0.000416	9.730253	0.260253	1.041537	-0.016772	-1.390288
21	H	0.000000	0.260253	0.533101	0.019403	-0.004182	0.005362
22	C	0.000004	1.041537	0.019403	7.092713	0.310709	0.301104
23	H	0.000000	-0.016772	-0.004182	0.310709	0.522195	-0.028464
24	C	-0.000006	-1.390288	0.005362	0.301104	-0.028464	8.801201
25	H	0.000000	0.021680	-0.000156	-0.039421	-0.004162	0.327072
26	C	-0.000195	2.685094	-0.022797	0.915808	0.005227	-4.694324
27	H	0.000000	-0.007213	0.000018	0.021636	-0.000148	0.052122
28	C	0.000962	-0.278692	0.001586	-0.043836	0.000001	0.038304
29	C	-0.000963	0.000735	-0.000484	-0.028434	-0.000060	0.071740

This journal is © The Royal Society of Chemistry 2014

30	O	-0.000007	0.018634	0.000000	0.003249	0.000000	-0.002565
31	O	0.000004	0.002268	0.000000	0.000510	0.000000	-0.002934
32	O	-0.000026	0.022189	0.000002	0.000475	0.000000	-0.000585
33	C	0.000124	-0.845999	0.002841	-0.160352	0.000383	0.527976
34	N	-0.000002	0.011555	-0.000007	-0.006392	0.000001	0.014750

		25	26	27	28	29	30
1	C	0.008410	1.076222	0.031295	-0.631759	-0.382950	0.003876
2	C	0.002886	-0.473888	-0.005280	0.733013	0.757167	0.121178
3	H	0.000000	0.012113	0.000002	-0.018533	-0.000687	-0.000407
4	C	0.024285	-11.075114	-0.105548	-0.462526	-0.373705	-0.015610
5	C	0.000716	-0.226071	-0.001028	-1.162527	0.472636	-0.349572
6	H	0.000000	-0.004609	0.000000	-0.073703	0.010374	0.005176
7	C	0.000747	0.487094	0.001969	-0.716648	-0.195473	-0.099533
8	C	-0.004429	3.316200	0.021271	-0.953355	-0.801314	-0.156964
9	C	-0.012392	-0.504420	-0.041983	1.029267	-0.028397	0.075220
10	C	-0.000360	0.079001	-0.001109	0.330391	-0.893692	-0.181950
11	H	0.000001	-0.050291	-0.000060	0.024542	-0.076758	0.004787
12	C	-0.000197	-0.430130	0.001009	0.333605	0.231079	0.018292
13	H	0.000000	0.000177	0.000000	0.015128	-0.000978	-0.000115
14	C	0.000714	-2.383206	-0.006519	0.638549	0.211640	0.036676
15	H	0.000000	-0.006707	0.000001	-0.000446	0.014474	-0.000112
16	C	0.000005	-0.003664	-0.000724	-0.030794	-0.034999	-0.015567
17	H	0.000000	0.000738	0.000000	-0.001163	0.001451	-0.000006
18	C	0.000010	-0.108031	-0.000024	0.043475	0.042679	0.009731
19	H	0.000000	-0.000195	0.000000	0.000962	-0.000963	-0.000007
20	C	0.021680	2.685094	-0.007213	-0.278692	0.000735	0.018634

This journal is © The Royal Society of Chemistry 2014

21	H	-0.000156	-0.022797	0.000018	0.001586	-0.000484	0.000000
22	C	-0.039421	0.915808	0.021636	-0.043836	-0.028434	0.003249
23	H	-0.004162	0.005227	-0.000148	0.000001	-0.000060	0.000000
24	C	0.327072	-4.694324	0.052122	0.038304	0.071740	-0.002565
25	H	0.519049	-0.027015	-0.003925	-0.000074	0.000000	0.000000
26	C	-0.027015	19.966354	0.333380	-0.191447	-0.020849	0.012141
27	H	-0.003925	0.333380	0.500865	-0.000497	0.002157	0.000000
28	C	-0.000074	-0.191447	-0.000497	6.708758	-0.726461	0.224519
29	C	0.000000	-0.020849	0.002157	-0.726461	6.354088	0.285372
30	O	0.000000	0.012141	0.000000	0.224519	0.285372	8.354217
31	O	0.000000	0.001071	0.000003	0.027518	0.512877	-0.067910
32	O	0.000000	0.004469	0.000000	0.433607	0.030862	-0.080112
33	C	-0.004637	-2.286170	-0.008962	0.347785	0.299798	0.030398
34	N	0.000139	-0.023404	0.004241	-0.001128	0.000538	-0.000701

		31	32	33	34
1	C	0.024122	0.022085	-4.025851	0.088373
2	C	-0.065776	-0.117870	-1.175127	0.059525
3	H	0.000070	0.004768	0.008266	-0.000025
4	C	0.020843	0.016659	0.203856	-0.098836
5	C	-0.029622	-0.004389	-0.467586	0.023111
6	H	-0.000619	-0.002207	0.013076	-0.000151
7	C	-0.012435	0.125529	-2.376059	0.112415
8	C	0.192631	0.073584	-3.330028	-0.175186
9	C	-0.022244	-0.052777	-4.978461	0.133196
10	C	-0.141103	-0.061644	-1.438930	-0.027000
11	H	-0.000785	-0.000652	0.007365	0.001346
12	C	-0.011009	-0.083264	0.539649	0.011776
13	H	0.000000	-0.000334	0.004116	-0.000002
14	C	-0.127331	-0.034214	2.491391	0.053761
15	H	-0.000363	-0.000001	0.010405	0.005572
16	C	-0.014113	0.001571	-0.166509	0.018492
17	H	-0.000040	0.000003	-0.005690	0.000088
18	C	-0.005567	-0.015223	0.051091	0.003749
19	H	0.000004	-0.000026	0.000124	-0.000002
20	C	0.002268	0.022189	-0.845999	0.011555
21	H	0.000000	0.000002	0.002841	-0.000007
22	C	0.000510	0.000475	-0.160352	-0.006392
23	H	0.000000	0.000000	0.000383	0.000001

This journal is © The Royal Society of Chemistry 2014

```
   24  C   -0.002934  -0.000585   0.527976   0.014750
   25  H    0.000000   0.000000  -0.004637   0.000139
   26  C    0.001071   0.004469  -2.286170  -0.023404
   27  H    0.000003   0.000000  -0.008962   0.004241
   28  C    0.027518   0.433607   0.347785  -0.001128
   29  C    0.512877   0.030862   0.299798   0.000538
   30  O   -0.067910  -0.080112   0.030398  -0.000701
   31  O    8.053432   0.000202   0.011129  -0.002912
   32  O    0.000202   8.102839  -0.011968   0.000084
   33  C    0.011129  -0.011968  22.472137   0.284619
   34  N   -0.002912   0.000084   0.284619   6.839010
Mulliken atomic charges:
             1
    1  C   -0.545054
    2  C    0.602338
    3  H    0.215727
    4  C    0.215812
    5  C   -0.394153
    6  H    0.256788
    7  C   -0.347812
    8  C    0.095770
    9  C    0.253549
   10  C   -0.002118
   11  H    0.271014
   12  C    0.307653
   13  H    0.191258
   14  C   -0.254894
   15  H    0.213167
   16  C   -0.439980
   17  H    0.191918
   18  C   -0.251765
   19  H    0.189804
   20  C    0.186520
   21  H    0.186435
   22  C   -0.287792
   23  H    0.189304
   24  C   -0.411368
   25  H    0.191056
   26  C   -0.362755
   27  H    0.213052
   28  C    0.362577
   29  C    0.266535
   30  O   -0.232337
   31  O   -0.341917
   32  O   -0.373659
   33  C   -0.024076
   34  N   -0.330596
Sum of Mulliken atomic charges =   0.00000
Mulliken charges with hydrogens summed into heavy atoms:
             1
    1  C   -0.545054
    2  C    0.818065
```

This journal is © The Royal Society of Chemistry 2014

```
     4  C    0.215812
     5  C   -0.137364
     7  C   -0.347812
     8  C    0.095770
     9  C    0.253549
    10  C    0.268896
    12  C    0.498911
    14  C   -0.041727
    16  C   -0.248061
    18  C   -0.061961
    20  C    0.372954
    22  C   -0.098489
    24  C   -0.220312
    26  C   -0.149703
    28  C    0.362577
    29  C    0.266535
    30  O   -0.232337
    31  O   -0.341917
    32  O   -0.373659
    33  C   -0.024076
    34  N   -0.330596
 Sum of Mulliken charges with hydrogens summed into heavy atoms =
0.00000
 Electronic spatial extent (au):  <R**2>=           5253.6605
 Charge=              0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=             -4.2891    Y=             -3.9017    Z=
1.6240  Tot=              6.0214
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=           -134.3785   YY=           -148.3110   ZZ=           -
125.1357
   XY=              5.4116   XZ=             12.5581   YZ=
1.3482
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=              1.5633   YY=            -12.3693   ZZ=
10.8060
   XY=              5.4116   XZ=             12.5581   YZ=
1.3482
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=            -69.9424  YYY=            -80.1659  ZZZ=
-13.5544  XYY=            -18.4611
  XXY=              1.4246  XXZ=             28.7613  XZZ=
31.9287  YZZ=             -0.8858
  YYZ=             30.1058  XYZ=             -0.7662
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=          -3230.2382 YYYY=          -2308.8283 ZZZZ=          -
1698.1207 XXXY=             30.3676
 XXXZ=             42.3221 YYYX=            103.0949 YYYZ=
10.2508 ZZZX=             58.2580
 ZZZY=             14.0194 XXYY=           -927.3871 XXZZ=           -
892.5797 YYZZ=           -634.7917
```

This journal is © The Royal Society of Chemistry 2014

XXYZ= -13.9883 YYXZ= 57.1133 ZZXY=
-7.7877
N-N= 1.879139480109D+03 E-N=-6.106342923359D+03 KE=
1.001752807065D+03
1|1|UNPC-MECHANOCHEM2|FOpt|RB3LYP|6-31+G(d)|C19H11N1O3|JAMES|24-Jul-
20
13|0||# opt b3lyp/6-31+g(d) geom=connectivity||9-
cyanoDAproduct||0,1|C
,-1.6571344215,-1.0634444331,-0.0250401127|C,-0.2282440624,-
1.57356063
62,-0.0408140537|H,-0.1612993862,-2.6620827867,0.0240503706|C,-
1.75812
26114,0.3359702463,-0.0961158008|C,0.3665261823,-1.0693455441,-
1.40333
64203|H,-0.178057295,-1.5447960167,-2.2247457414|C,0.5295305178,-
0.873
7445765,1.0735194949|C,0.4455409465,0.5285377129,1.028489438|C,-
0.3869
167394,1.0347334612,-0.1577888609|C,0.3100293552,0.4703669465,-
1.46861
75063|H,-0.2377321684,0.8406326582,-2.3401896912|C,1.2704626784,-
1.494
4549168,2.0772931164|H,1.3453182135,-
2.5787358392,2.1092617194|C,1.094

4438091,1.3126513143,1.9787395917|H,1.0342407089,2.3965438037,1.934054

8618|C,1.8295166344,0.6829834862,2.9909507497|H,2.3366811748,1.2863378
745,3.7386644557|C,1.9177962969,-
0.7102248803,3.0399442755|H,2.4940312
208,-1.1900491297,3.8263252532|C,-2.8087719671,-
1.8440841288,0.0348646
378|H,-2.7322515107,-2.927680747,0.0897238443|C,-4.0643091559,-
1.22210
10005,0.0310111794|H,-4.9656596606,-1.826653325,0.085218461|C,-
4.15985
61443,0.1691765005,-0.0390315379|H,-5.1351489611,0.6480260552,-
0.03925
43013|C,-3.0034938921,0.9581325689,-0.1059121584|H,-
3.079910823,2.0407
310323,-0.1572165078|C,1.8420158178,-1.4043624855,-
1.5544410448|C,1.77
14292148,0.8936549502,-1.6092781528|O,2.5823190215,-0.2360556267,-
1.66
56838527|O,2.228680685,1.9959559468,-1.68535536|O,2.36027375,-
2.484402
4018,-1.5833025473|C,-0.5163169185,2.4930402201,-0.1978427521|N,-
0.672
50851,3.6429126966,-0.2108150469||Version=IA32W-G09RevA.02|State=1-
A|H
F=-1011.1115461|RMSD=1.911e-009|RMSF=1.846e-005|Dipole=-1.6834491,-
1.5

```
 465253,0.6216305|Quadrupole=1.3255935,-
9.2354099,7.9098164,3.8302919,9
 .4733828,0.612064|PG=C01 [X(C19H11N1O3)]||@


 IT PROBABLY IS NOT POSSIBLE FOR A SCIENTIST TO INTERROGATE NATURE
 FROM A WHOLLY DISINTERESTED VIEWPOINT.
 EVEN IF HE HAS NO PARTICULAR AXE TO GRIND, HE IS LIKELY TO HAVE
 A DISTINCTIVE WAY OF VIEWING NATURE.

                                                 -- JOHN LOSEE
 Job cpu time:  0 days  5 hours 40 minutes 35.0 seconds.
 File lengths (MBytes):  RWF=    131 Int=      0 D2E=      0 Chk=
13 Scr=      1
 Normal termination of Gaussian 09 at Wed Jul 24 03:28:42 2013.
```