Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
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  |  Jaguar version 3.5, release  42
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|
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|
  |  Use of this program should be acknowledged in publications as:
|
  |  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.
|
  +-----------------------------------------------------------------
--+

  start of program pre
  Job name: WF26536
  Executables used: C:\USERS\GIANCARLO\GOOGLE
  Temporary files : DRIVE\1.

  Input file comments:
    Molecule001
    This file created by Spartan

  basis set:             6-31G**
  net molecular charge:    0
  multiplicity:            1

  number of basis functions....          375

 Input geometry:
                                 angstroms
  atom            x                   y                   z
  C10       0.4357510000      0.1832390000     -1.5127670000
  C1        0.7742270000      0.2659640000     -0.0963000000
  H2       -1.2029670000     -0.1536590000      0.6696490000
  C2       -0.1531660000      0.0706740000      0.9218030000
  C3        2.5315980000      0.6533160000      1.5820370000
  C4        0.2271680000      0.1513410000      2.2692830000
  C5        2.1168510000      0.5732050000      0.2493210000
  C6        1.5743070000      0.4353910000      2.5837220000
  C7       -0.7030100000     -0.0448790000      3.3525840000
  C8       -0.2742860000      0.0419660000      4.6282810000
  H6       -1.7537850000     -0.2628330000      3.1041150000
```

```
  H7       -0.9309380000     -0.0964640000      5.4992220000
  C9        1.1203330000      0.3320870000      4.9261680000
  O2        1.6805300000      0.4452200000      6.0146870000
  O1        2.0285850000      0.5248890000      3.8799640000
  H13       3.5757630000      0.8783000000      1.8400280000
  O3        3.1047290000      0.7621910000     -0.6887030000
  C11       1.3539090000      0.5723840000     -2.4201670000
  C13      -0.8757150000     -0.3218640000     -1.9224450000
  C12       2.6879200000      1.0788380000     -2.0253410000
  H22       1.1549410000      0.5419510000     -3.5014300000
  H23       2.7202020000      2.2006900000     -2.1217190000
  H24       3.5004730000      0.6242620000     -2.6587850000
  C14      -3.3660920000     -1.2937710000     -2.7545210000
  C15      -1.3325880000     -1.5703330000     -1.4775400000
  C16      -1.6758400000      0.4331850000     -2.7910060000
  C17      -2.9166030000     -0.0511740000     -3.2007830000
  C18      -2.5713040000     -2.0526050000     -1.8951140000
  H1       -0.7039670000     -2.1713440000     -0.8025700000
  H3       -1.3208010000      1.4124500000     -3.1452270000
  H4       -3.5408550000      0.5489730000     -3.8791690000
  H5       -2.9208650000     -3.0359650000     -1.5464000000
  H8       -4.3445110000     -1.6756250000     -3.0808770000

  Molecular weight:    276.08 amu

  Stoichiometry:        C18H12O3
  Molecular Point Group: C1
  Point Group used: C1
  nuclear repulsion energy.......  1510.120695165 hartrees

 Non-default options chosen:
   Geometry will be optimized in redundant internal coordinates
   Initial Hessian: from previous calculation

  end of program pre


  start of program onee
  smallest eigenvalue of S:    3.253E-04
  number of canonical orbitals.....          373
  end of program onee


  start of program hfig
  initial wavefunction generated automatically from atomic
wavefunctions

  Irreducible     Total no   No of occupied orbitals
```

```
representation  orbitals   Shell_1  Shell_2    ...
No Symm          373         72
------------------------
Orbital occupation/shell    1.000

end of program hfig


start of program probe
end of program probe


start of program grid

number of gridpoints:
   atom       C10     C1     H2     C2     C3     C4     C5     C6
grid # 1       90     87     71     88     89     91     87     85
grid # 2       98     96    114     96     97     99     96     93
grid # 3      192    197    203    185    186    200    185    186
grid # 4      336    340    209    330    333    349    315    322

number of gridpoints:
   atom        C7     C8     H6     H7     C9     O2     O1    H13
grid # 1       86     85     73     73     83    111    110     73
grid # 2       93     94    118    118     93    123    119    118
grid # 3      187    187    216    224    171    270    250    224
grid # 4      331    333    224    232    299    473    444    230

number of gridpoints:
   atom        O3    C11    C13    C12    H22    H23    H24    C14
grid # 1      111     88     91     80     71     71     71     89
grid # 2      119     96     99     90    114    111    113     97
grid # 3      253    184    195    162    219    222    221    187
grid # 4      446    332    343    289    226    227    227    331

number of gridpoints:
   atom       C15    C16    C17    C18     H1     H3     H4     H5
grid # 1       88     88     89     89     71     71     73     73
grid # 2       96     95     97     96    115    115    118    118
grid # 3      184    184    186    185    219    219    224    224
grid # 4      329    330    330    330    224    225    232    232

number of gridpoints:
   atom        H8  total
grid # 1       73   2769
grid # 2      118   3472
grid # 3      224   6755
grid # 4      232   9985
```

```
 end of program grid


 start of program rwr
 end of program rwr


 start of program scf
number of electrons.........        144
number of alpha electrons....         72
number of beta electrons.....         72
number of orbitals, total....        373
number of core orbitals......         72
number of open shell orbs....          0
number of occupied orbitals..         72
number of virtual orbitals...        301
number of hamiltonians.......          1
number of shells.............          1
SCF type: HF

      i  u  d  i  g                                          RMS    maximum
      t  p  i  c  r                          energy  density   DIIS
      e  d  i  u  i      total energy        change  change    error

etot  1  N  N  5  M  -910.21666520308                  4.6E-03  1.5E-01
etot  2  Y  Y  6  M  -912.88595463096  2.7E+00         1.8E-03  7.3E-02
etot  3  Y  Y  6  M  -913.13737267583  2.5E-01         7.3E-04  4.3E-02
etot  4  N  Y  2  U  -913.18777122062  5.0E-02         5.2E-04  1.8E-02
etot  5  Y  Y  6  M  -913.19693502452  9.2E-03         1.3E-03  1.2E-02
etot  6  N  Y  2  U  -913.20476585040  7.8E-03         1.6E-04  2.5E-03
etot  7  Y  Y  6  M  -913.20515394837  3.9E-04         6.8E-05  7.1E-04
etot  8  Y  Y  6  M  -913.20523340549  7.9E-05         1.3E-05  2.3E-04
etot  9  N  Y  2  U  -913.20515536868 -7.8E-05         8.4E-06  1.1E-04
etot 10  Y  Y  6  M  -913.20515826065  2.9E-06         4.9E-06  3.5E-05
etot 11  Y  N  6  M  -913.20516076141  2.5E-06         0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1510.12069516477
   (E)  Total one-electron terms..... -4242.83594488963
   (I)  Total two-electron terms.....  1819.51008896346
   (L)  Electronic energy............. -2423.32585592617  (E+I)
   (N)  Total energy.................  -913.20516076141  (A+L)

 SCFE: SCF energy: HF    -913.20516076141 hartrees   iterations:  11
```

```
HOMO energy:    -0.28697
LUMO energy:     0.06700

 Orbital energies:
 -20.63185  -20.60745  -20.53598  -11.38849  -11.33592  -11.33283
 -11.31208  -11.29365  -11.27363  -11.26479  -11.26155  -11.25986
 -11.25978  -11.25860  -11.25282  -11.25235  -11.25215  -11.25159
 -11.25109  -11.25021  -11.24766   -1.46405   -1.42071   -1.34452
  -1.18785   -1.16806   -1.12538   -1.11029   -1.03890   -1.03278
  -1.02476   -1.02049   -0.93322   -0.89392   -0.87805   -0.86159
  -0.83612   -0.82751   -0.78669   -0.73725   -0.72686   -0.71041
  -0.68524   -0.68157   -0.66618   -0.65794   -0.64729   -0.64129
  -0.63695   -0.63184   -0.61245   -0.60233   -0.59451   -0.59105
  -0.58675   -0.57883   -0.54774   -0.53896   -0.52371   -0.51761
  -0.51270   -0.50210   -0.50062   -0.49129   -0.47610   -0.44441
  -0.43864   -0.38771   -0.34978   -0.34405   -0.32753   -0.28697
   0.06700    0.08957    0.12050    0.12745    0.15468    0.20730
   0.22351    0.22867    0.23850    0.25984

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  17    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    C10     2.916770E-02   1.074906E-02  -2.798132E-02
  2    C1      8.999028E-03   2.205580E-03   1.559231E-02
  3    H2      2.042971E-02   5.162653E-03   5.998974E-03
  4    C2      3.974762E-04   1.677696E-03  -9.242467E-04
  5    C3     -7.164929E-03  -1.576973E-03  -1.518284E-03
  6    C4      1.241098E-02   2.782811E-03  -5.231884E-03
  7    C5      2.014092E-02   1.942718E-03   6.664503E-03
  8    C6      1.466640E-02   3.474338E-03   7.177619E-04
  9    C7     -4.635896E-03  -9.675423E-04   1.481055E-02
 10    C8     -1.791523E-02  -3.734257E-03   3.291916E-03
```

11	H6	1.683825E-02	3.472495E-03	6.789925E-03
12	H7	1.228038E-02	2.577919E-03	-1.539383E-02
13	C9	8.717321E-02	1.795750E-02	5.583692E-02
14	O2	-5.762859E-02	-1.175894E-02	-5.606745E-02
15	O1	-5.534046E-02	-1.145966E-02	-2.188651E-02
16	H13	-1.845024E-02	-3.927563E-03	-4.793097E-03
17	O3	-4.007071E-02	-5.487638E-03	5.118904E-03
18	C11	-2.541979E-02	-1.276401E-02	3.414058E-03
19	C13	-1.991052E-02	-5.445653E-03	-1.067803E-02
20	C12	3.898664E-02	1.571113E-02	-1.676969E-03
21	H22	1.276307E-03	-1.438188E-03	1.736769E-02
22	H23	2.427076E-03	-2.307947E-02	-1.658461E-03
23	H24	-2.116158E-02	1.547838E-02	1.087154E-02
24	C14	-7.437388E-03	-1.828324E-03	-3.088247E-03
25	C15	7.216648E-04	-4.845033E-03	1.868705E-03
26	C16	5.964351E-04	3.294244E-03	-1.675059E-03
27	C17	-5.228342E-03	3.142618E-03	-5.769273E-03
28	C18	-1.605187E-03	-7.698077E-03	3.154365E-03
29	H1	-1.047515E-02	9.385674E-03	-1.173481E-02
30	H3	-5.933306E-03	-1.553493E-02	6.817855E-03
31	H4	9.592431E-03	-9.360433E-03	1.063314E-02
32	H5	5.553480E-03	1.536652E-02	-5.637283E-03
33	H8	1.515776E-02	6.000173E-03	5.210168E-03
total		-1.561441E-03	-5.251818E-04	-1.555476E-03

```
 end of program der1b


 start of program geopt   1

 geometry optimization step  1
 reading input hessian of dimension    99
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3007162
  Cos(theta):   0.9150272

  Final level shift:  -9.7502445E-02

 gradient maximum:        7.6908E-02 .  (  4.5000E-04 )
 gradient rms:            1.4007E-02 .  (  3.0000E-04 )
 step size:   0.30071  trust radius:   0.30000
 displacement maximum:    1.1516E-01 .  (  1.8000E-03 )
 displacement rms:        2.6789E-02 .  (  1.2000E-03 )
```

```
  predicted energy change:    -2.6039E-02    geom step:   3.0071E-01
full step:   3.0071E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.0577E-02     y:     5.0120E-03     z:    -4.4406E-05

  new geometry:
                                angstroms
  atom            x                 y                 z
  C10        0.4512124238      0.1688457941     -1.5224329939
  C1         0.7921211215      0.2615808321     -0.0842264455
  H2        -1.1472972907     -0.1513504583      0.7031670991
  C2        -0.1207490422      0.0706080601      0.9409234318
  C3         2.5256907049      0.6553431718      1.5848621593
  C4         0.2485104596      0.1519224795      2.2784662912
  C5         2.1238891844      0.5709004600      0.2658257701
  C6         1.5810566024      0.4417288441      2.5884625579
  C7        -0.6608260819     -0.0432468202      3.3794325905
  C8        -0.2327746255      0.0577976746      4.6382051063
  H6        -1.6947195809     -0.2676825112      3.1644362932
  H7        -0.8697956689     -0.0757161094      5.4982047633
  C9         1.1693212088      0.3650867061      4.9347668341
  O2         1.5826151267      0.4756991106      6.0340850771
  O1         2.0052150834      0.5396750483      3.8716656224
  H13        3.5500170868      0.8803469990      1.8346530330
  O3         3.0729754986      0.7514822167     -0.6686642012
  C11        1.3646937940      0.5548066839     -2.4105102366
  C13       -0.8866349883     -0.3360836769     -1.9487296385
  C12        2.7056901839      1.0739109465     -2.0071470736
  H22        1.1726155090      0.5060162330     -3.4721969872
  H23        2.7642184645      2.1625823825     -2.1356069458
  H24        3.4833437420      0.6241836289     -2.6318819608
  C14       -3.3759421929     -1.2949218331     -2.7848093406
  C15       -1.3388323708     -1.5919161542     -1.5406455408
  C16       -1.6951446294      0.4274012147     -2.7831937736
  C17       -2.9316600927     -0.0465596132     -3.2011715896
  C18       -2.5744384187     -2.0693314804     -1.9533894569
  H1        -0.7074474452     -2.2013439794     -0.9164164643
  H3        -1.3641089044      1.4019728594     -3.0805857235
  H4        -3.5566692396      0.5583252160     -3.8314782788
  H5        -2.9109358054     -3.0482514011     -1.6356097056
  H8        -4.3405179107     -1.6613352236     -3.1076847407

  nuclear repulsion energy.......  1515.070753123 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   1   /
 ------------------------------------------------
```

```
end of program geopt


start of program onee
smallest eigenvalue of S:    2.977E-04
number of canonical orbitals.....          373
end of program onee


start of program probe
end of program probe


start of program grid

number of gridpoints:
   atom       C10     C1      H2      C2      C3      C4      C5      C6
grid # 1       92     89      71      86      89      88      86      85
grid # 2      100     99     115      96      97      99      94      95
grid # 3      192    199     203     183     184     201     182     184
grid # 4      340    346     203     327     330     348     315     314

number of gridpoints:
   atom        C7     C8      H6      H7      C9      O2      O1     H13
grid # 1       86     88      73      73      79     111     108      73
grid # 2       93     95     118     118      89     123     118     118
grid # 3      186    185     217     224     170     270     248     224
grid # 4      326    333     218     223     285     467     442     222

number of gridpoints:
   atom        O3    C11     C13     C12     H22     H23     H24     C14
grid # 1      110     87      91      77      71      71      70      89
grid # 2      119     94     100      89     114     112     112      97
grid # 3      250    180     195     158     219     222     218     185
grid # 4      444    327     338     283     218     226     224     327

number of gridpoints:
   atom       C15    C16     C17     C18      H1      H3      H4      H5
grid # 1       87     87      89      89      71      71      73      73
grid # 2       96     95      97      96     115     115     118     118
grid # 3      183    183     185     184     218     218     223     224
grid # 4      328    329     329     329     218     218     224     224

number of gridpoints:
   atom        H8  total
grid # 1       73   2756
grid # 2      118   3472
```

```
 grid # 3      223   6720
 grid # 4      224   9849

 end of program grid


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  2  U  -913.21155876481             4.0E-04  8.8E-03
etot  2  Y  Y  6  M  -913.22641842379  1.5E-02    1.3E-04  2.8E-03
etot  3  N  Y  2  U  -913.22778691100  1.4E-03    4.9E-05  1.1E-03
etot  4  Y  Y  6  M  -913.22803207910  2.5E-04    2.1E-05  3.7E-04
etot  5  Y  Y  6  M  -913.22806740979  3.5E-05    7.6E-06  1.4E-04
etot  6  Y  Y  6  M  -913.22807567467  8.3E-06    3.1E-06  4.6E-05
etot  7  Y  N  6  M  -913.22807758956  1.9E-06    0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1515.07075312255
   (E)  Total one-electron terms..... -4252.64946376541
   (I)  Total two-electron terms.....  1824.35063305330
   (L)  Electronic energy............. -2428.29883071211  (E+I)
   (N)  Total energy.................  -913.22807758956  (A+L)

 SCFE: SCF energy: HF    -913.22807758956 hartrees   iterations:   7


 HOMO energy:    -0.28739
 LUMO energy:     0.08229

  Orbital energies:
  -20.63255  -20.60418  -20.54057  -11.38153  -11.33136  -11.32547
  -11.30720  -11.27650  -11.26427  -11.26358  -11.25608  -11.25436
  -11.25239  -11.24689  -11.24660  -11.24544  -11.24507  -11.24487
  -11.24442  -11.24357  -11.23941   -1.48444   -1.43278   -1.38300
   -1.18643   -1.16966   -1.12158   -1.11133   -1.04318   -1.03465
   -1.02636   -1.02028   -0.93785   -0.89917   -0.87613   -0.86339
   -0.83981   -0.83197   -0.79330   -0.74333   -0.72854   -0.71337
```

```
  -0.68904   -0.68742   -0.67146   -0.66457   -0.66082   -0.64432
  -0.63866   -0.63294   -0.61843   -0.61209   -0.59734   -0.59338
  -0.58947   -0.57987   -0.55361   -0.54270   -0.52538   -0.51595
  -0.51368   -0.50984   -0.50240   -0.49510   -0.46993   -0.44159
  -0.44118   -0.38970   -0.34816   -0.34391   -0.32687   -0.28739
   0.08229    0.09640    0.12566    0.13100    0.16596    0.21154
   0.23106    0.24141    0.24548    0.26912

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    C10     5.583508E-03   3.106099E-03  -5.165140E-03
  2    C1     -1.052063E-04   1.575574E-04   5.066899E-03
  3    H2      2.275832E-03   7.324116E-04   4.400547E-04
  4    C2      1.948392E-03   9.853129E-04  -6.545237E-03
  5    C3     -4.335519E-03  -1.135048E-03   8.655024E-03
  6    C4      1.209040E-02   2.804192E-03   1.871452E-03
  7    C5     -1.028457E-03  -9.966184E-04  -2.261382E-03
  8    C6      3.137986E-03   1.179437E-03  -7.669662E-03
  9    C7     -5.670024E-03  -6.121499E-04   6.758296E-03
 10    C8     -3.902183E-03  -1.801476E-03  -3.444714E-03
 11    H6      2.085378E-03   4.204867E-04   6.294599E-04
 12    H7      3.010185E-03   6.066332E-04  -4.104963E-03
 13    C9     -8.018253E-03   3.871076E-04  -4.914014E-03
 14    O2      1.103543E-02   1.532791E-03   3.975380E-03
 15    O1     -6.676625E-03  -2.198698E-03   3.859042E-04
 16    H13    -4.028019E-03  -6.882326E-04  -1.174017E-03
 17    O3     -6.419762E-03   5.118435E-04  -4.809680E-03
 18    C11    -8.037853E-03  -3.338174E-03   2.359674E-03
 19    C13    -8.693819E-04  -3.099082E-03  -8.497357E-04
 20    C12     1.121042E-02   9.991985E-04   1.092542E-03
 21    H22    -4.040073E-04  -4.679630E-04   3.140904E-03
 22    H23    -4.295993E-04  -5.801171E-03   1.514104E-03
```

23	H24	-4.898012E-03	4.567906E-03	4.260826E-03
24	C14	-2.820637E-04	6.919352E-04	-8.966144E-04
25	C15	-1.056946E-03	-1.280472E-03	-2.026571E-03
26	C16	-3.008021E-03	-2.032519E-03	1.576360E-03
27	C17	8.102599E-05	-4.388681E-03	3.676443E-03
28	C18	-8.745572E-05	-1.101381E-03	-5.434020E-04
29	H1	-1.375205E-03	2.713185E-04	1.391319E-04
30	H3	6.666352E-04	2.708325E-03	-1.700593E-03
31	H4	2.661461E-04	1.059843E-03	-1.243958E-03
32	H5	2.054686E-03	4.660961E-03	-1.216580E-03
33	H8	3.611233E-03	1.182264E-03	1.445501E-03
total		-1.575320E-03	-3.760424E-04	-1.578307E-03

end of program der1b

start of program geopt 2

geometry optimization step 2
reading input hessian of dimension 99
in five columns format

energy change: -2.2917E-02 . (5.0000E-05)
gradient maximum: 1.9961E-02 . (4.5000E-04)
gradient rms: 3.3667E-03 . (3.0000E-04)
step size: 0.25542 trust radius: 0.30000
displacement maximum: 1.1645E-01 . (1.8000E-03)
displacement rms: 2.2755E-02 . (1.2000E-03)
predicted energy change: -2.0854E-03 geom step: 2.5542E-01
full step: 2.5542E-01
molecular structure not yet converged...

center of mass moved by:
x: 2.8510E-03 y: -1.6883E-02 z: -1.7463E-04

new geometry:

		angstroms	
atom	x	y	z
C10	0.4392209799	0.1856751829	-1.5217711831
C1	0.7708351698	0.2902608670	-0.0793577309
H2	-1.1717642266	-0.0216863582	0.7087102752
C2	-0.1402835425	0.1546543374	0.9415457632
C3	2.5228217163	0.6106688595	1.5917780330
C4	0.2410166620	0.2190263312	2.2841114611
C5	2.1113981575	0.5430694305	0.2713760251
C6	1.5801712550	0.4420633833	2.5854784458

```
 C7       -0.6742001692      0.0556667905      3.3990022104
 C8       -0.2302799943      0.1146950692      4.6535777529
 H6       -1.7135964765     -0.1186263482      3.1879011569
 H7       -0.8584287078     -0.0006148542      5.5109933159
 C9        1.1878472177      0.3524884520      4.9460927421
 O2        1.6677534875      0.4176357095      6.0230418187
 O1        2.0024818480      0.4994950957      3.8678272576
 H13       3.5507348814      0.7879775183      1.8340651253
 O3        3.0575748791      0.6788017974     -0.6700027776
 C11       1.3540882069      0.5545324339     -2.4031589848
 C13      -0.8952391538     -0.3334195672     -1.9503842104
 C12       2.6955341114      1.0814805320     -1.9858429893
 H22       1.1698212453      0.4890907878     -3.4588902188
 H23       2.7259372517      2.1752020993     -2.0442724865
 H24       3.4734046586      0.7005081911     -2.6395155375
 C14      -3.3654889785     -1.3216522287     -2.8072815539
 C15      -1.3152205255     -1.6100131581     -1.5845420996
 C16      -1.7286421163      0.4381339273     -2.7505683550
 C17      -2.9575121622     -0.0539270757     -3.1752993605
 C18      -2.5376750181     -2.0995192043     -2.0182317001
 H1       -0.6743269994     -2.2275518880     -0.9725617572
 H3       -1.4168582416      1.4311688628     -3.0429567174
 H4       -3.5891265153      0.5614952719     -3.8029006529
 H5       -2.8343304910     -3.0900509565     -1.7506133278
 H8       -4.3127629303     -1.6994189314     -3.1435253747

 nuclear repulsion energy.......  1516.146086422 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   2   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.919E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       C10     C1      H2      C2      C3      C4      C5      C6
```

```
  grid # 1       92     90     71     86     89     93     87     89
  grid # 2      100     98    115     96     97    101     94     97
  grid # 3      192    198    208    181    183    199    182    184
  grid # 4      340    340    204    328    328    341    311    308

  number of gridpoints:
     atom        C7     C8     H6     H7     C9     O2     O1    H13
  grid # 1       85     88     73     73     79    111    108     73
  grid # 2       93     95    118    118     89    123    118    118
  grid # 3      186    185    218    224    169    270    248    224
  grid # 4      326    333    218    223    286    467    443    222

  number of gridpoints:
     atom        O3    C11    C13    C12    H22    H23    H24    C14
  grid # 1      111     87     92     79     72     70     70     89
  grid # 2      120     94    100     89    114    112    112     97
  grid # 3      250    182    195    157    220    222    218    184
  grid # 4      443    324    340    284    219    226    223    328

  number of gridpoints:
     atom       C15    C16    C17    C18     H1     H3     H4     H5
  grid # 1       88     87     89     89     72     72     73     73
  grid # 2       96     95     97     96    115    115    118    118
  grid # 3      184    183    183    184    219    219    223    222
  grid # 4      327    326    327    327    219    218    224    224

  number of gridpoints:
     atom        H8  total
  grid # 1       73   2773
  grid # 2      118   3476
  grid # 3      223   6719
  grid # 4      224   9821

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
       r  t  s  t  d     total energy   change  change    error

etot   1  N  N  2  U  -913.21248679035           3.0E-04  6.9E-03
```

```
etot   2  Y  Y  6  M  -913.22749400166  1.5E-02  1.3E-04  2.6E-03
etot   3  N  Y  2  U  -913.22940043296  1.9E-03  3.7E-05  6.5E-04
etot   4  Y  Y  6  M  -913.22952527069  1.2E-04  1.8E-05  3.0E-04
etot   5  Y  Y  6  M  -913.22955524403  3.0E-05  6.2E-06  1.2E-04
etot   6  Y  Y  6  M  -913.22955890201  3.7E-06  3.2E-06  5.7E-05
etot   7  Y  N  6  M  -913.22956003487  1.1E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1516.14608642233
   (E)  Total one-electron terms..... -4254.81593873146
   (I)  Total two-electron terms.....  1825.44029227425
   (L)  Electronic energy............. -2429.37564645721  (E+I)
   (N)  Total energy.................  -913.22956003487  (A+L)

 SCFE: SCF energy: HF    -913.22956003487 hartrees   iterations:   7


 HOMO energy:    -0.28993
 LUMO energy:     0.08200

  Orbital energies:
  -20.62825  -20.60330  -20.53984  -11.38135  -11.32768  -11.32468
  -11.30631  -11.27806  -11.26288  -11.26277  -11.25552  -11.25270
  -11.25193  -11.24522  -11.24502  -11.24477  -11.24468  -11.24381
  -11.24283  -11.24155  -11.23684   -1.48501   -1.43408   -1.38029
   -1.18724   -1.17074   -1.12205   -1.11237   -1.04494   -1.03655
   -1.02606   -1.02060   -0.93966   -0.89883   -0.87714   -0.86467
   -0.84000   -0.83205   -0.79364   -0.74513   -0.72932   -0.71437
   -0.69132   -0.68741   -0.67176   -0.66454   -0.66060   -0.64415
   -0.63832   -0.63398   -0.61888   -0.61430   -0.59574   -0.59440
   -0.59073   -0.58008   -0.55364   -0.54281   -0.52604   -0.51469
   -0.51291   -0.50953   -0.50235   -0.49342   -0.46678   -0.44223
   -0.44014   -0.39111   -0.34867   -0.34486   -0.32764   -0.28993
    0.08200    0.09970    0.12785    0.13186    0.16499    0.21130
    0.23115    0.24235    0.24805    0.27064

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr
```

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	C10	-2.415077E-03	-3.596675E-04	3.197521E-03
2	C1	5.139750E-03	1.651357E-03	-1.918400E-03
3	H2	-1.916664E-03	-3.999507E-04	-3.005319E-04
4	C2	-1.740224E-03	-1.157083E-03	6.249496E-03
5	C3	-5.516157E-04	1.766714E-04	-6.123009E-03
6	C4	-1.420135E-03	6.063688E-04	-5.348630E-04
7	C5	1.530547E-03	1.277084E-04	-4.044902E-04
8	C6	-4.163676E-03	-1.702017E-03	4.288094E-03
9	C7	3.377354E-03	4.827974E-04	-1.229130E-03
10	C8	1.389819E-03	9.255633E-04	4.025262E-04
11	H6	-1.229987E-03	-1.143177E-04	5.090731E-04
12	H7	-2.428545E-03	-4.860416E-04	1.339549E-03
13	C9	-1.523623E-03	-1.316116E-03	-8.380505E-03
14	O2	2.037714E-04	5.021861E-04	4.287122E-03
15	O1	1.060869E-03	8.803123E-04	-2.817966E-03
16	H13	1.269682E-03	2.444016E-04	-8.790796E-06
17	O3	2.358301E-04	1.148286E-03	-5.546668E-03
18	C11	2.780406E-03	1.300630E-03	-1.129485E-03
19	C13	1.197626E-03	2.208081E-04	-4.405831E-05
20	C12	2.213791E-04	1.835657E-03	4.441186E-03
21	H22	-1.100601E-03	-5.034844E-04	-1.606219E-03
22	H23	-4.905756E-04	-4.143235E-03	1.323903E-03
23	H24	-8.318394E-04	2.908243E-04	2.800304E-03
24	C14	-3.134318E-04	1.828283E-03	-2.289566E-03
25	C15	-3.626716E-04	-2.845252E-03	5.138697E-04
26	C16	-1.836177E-03	3.231368E-03	-2.805067E-03
27	C17	7.289717E-04	6.994275E-03	-3.415764E-03
28	C18	5.346228E-03	1.581687E-03	2.001457E-03
29	H1	-2.051656E-03	1.618205E-03	-1.824451E-03
30	H3	-1.280703E-03	-3.636914E-03	1.593088E-03
31	H4	2.390428E-03	-2.604408E-03	3.199456E-03
32	H5	-1.764508E-03	-5.417366E-03	2.421134E-03
33	H8	-1.163933E-03	-1.136634E-03	8.917732E-05
total		-1.712983E-03	-1.750976E-04	-1.722007E-03

end of program der1b

start of program geopt 3

```
  geometry optimization step  3
  reading input hessian of dimension    99
   in five columns format
  reading input hessian of dimension    99
   in five columns format


  energy change:          -1.4824E-03 .  (  5.0000E-05 )
  gradient maximum:        7.1625E-03 .  (  4.5000E-04 )
  gradient rms:            1.9852E-03 .  (  3.0000E-04 )
  step size:   0.12516  trust radius:   0.30000
  displacement maximum:    6.1507E-02 .  (  1.8000E-03 )
  displacement rms:        1.1150E-02 .  (  1.2000E-03 )
  predicted energy change:    -6.0084E-04    geom step:   1.2516E-01
full step:   1.2516E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.7980E-03     y:     6.2855E-03     z:    -6.0777E-03

  new geometry:
                              angstroms
  atom            x                y                z
  C10       0.4549611755     0.1651830248    -1.5210596501
  C1        0.7819223152     0.2810354256    -0.0809492674
  H2       -1.1657903370    -0.0511187709     0.6958179386
  C2       -0.1377422336     0.1387844632     0.9373079340
  C3        2.5152749123     0.6241527720     1.5884173688
  C4        0.2324464009     0.2178872797     2.2780697916
  C5        2.1170534122     0.5440562491     0.2674927154
  C6        1.5656461241     0.4527801352     2.5796649411
  C7       -0.6852452068     0.0559331152     3.3864157377
  C8       -0.2476222606     0.1245514798     4.6410108741
  H6       -1.7237600453    -0.1266483295     3.1772572289
  H7       -0.8822095728     0.0066706665     5.4942211226
  C9        1.1666299633     0.3685259490     4.9295388661
  O2        1.6447668431     0.4371875600     6.0096210481
  O1        1.9844501096     0.5255194290     3.8602614244
  H13       3.5397107838     0.8130364382     1.8368906556
  O3        3.0672190405     0.6806572603    -0.6688484379
  C11       1.3718456152     0.5231530147    -2.4051981035
  C13      -0.8827226107    -0.3472550145    -1.9472894374
  C12       2.7106217271     1.0549228132    -1.9847863176
  H22       1.1852425480     0.4460075916    -3.4610197375
  H23       2.7400775683     2.1423023586    -2.0616891155
  H24       3.4913062185     0.6623810153    -2.6175640193
  C14      -3.3590899373    -1.3092343161    -2.7866711436
  C15      -1.2830413112    -1.6439348020    -1.6244138398
```

```
 C16      -1.7400872430      0.4596372228     -2.6927497318
 C17      -2.9718369156     -0.0192812873     -3.1097220600
 C18      -2.5107242741     -2.1216194089     -2.0412454416
 H1       -0.6246929539     -2.2808458180     -1.0642421463
 H3       -1.4453150877      1.4673643813     -2.9349267643
 H4       -3.6268092782      0.6188385111     -3.6740408563
 H5       -2.8011225256     -3.1296756211     -1.7919931075
 H8       -4.3150589165     -1.6834064526     -3.1036199206

 nuclear repulsion energy.......  1517.834286134 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   3   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.897E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       C10     C1     H2     C2     C3     C4     C5     C6
 grid # 1       92     88     71     86     89     92     87     85
 grid # 2      100     96    115     96     97    101     94     95
 grid # 3      193    198    209    183    184    199    182    184
 grid # 4      340    344    204    327    328    340    310    314

 number of gridpoints:
    atom        C7     C8     H6     H7     C9     O2     O1    H13
 grid # 1       85     88     73     73     79    111    108     73
 grid # 2       93     95    118    118     89    123    118    118
 grid # 3      186    185    218    224    169    270    248    224
 grid # 4      326    333    218    224    286    467    443    222

 number of gridpoints:
    atom        O3    C11    C13    C12    H22    H23    H24    C14
 grid # 1      110     87     92     78     72     70     70     89
 grid # 2      120     94    100     85    114    111    112     97
 grid # 3      251    182    196    155    220    222    218    184
```

```
 grid # 4      443    324    341    283    219    226    219    327

 number of gridpoints:
    atom       C15    C16    C17    C18     H1     H3     H4     H5
 grid # 1       88     87     89     89     72     72     73     73
 grid # 2       96     95     97     96    115    115    118    118
 grid # 3      182    182    183    184    219    218    223    223
 grid # 4      327    328    328    328    219    218    224    224

 number of gridpoints:
    atom        H8  total
 grid # 1       73   2764
 grid # 2      118   3467
 grid # 3      223   6721
 grid # 4      224   9828

 end of program grid


 start of program rwr
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  2  U  -913.22404478262             1.6E-04  7.3E-03
etot  2  Y  Y  6  M  -913.22905491246  5.0E-03    7.7E-05  2.8E-03
etot  3  N  Y  2  U  -913.22981957671  7.6E-04    2.2E-05  8.7E-04
etot  4  Y  Y  6  M  -913.22987368374  5.4E-05    1.2E-05  2.7E-04
etot  5  Y  Y  6  M  -913.22988767803  1.4E-05    3.2E-06  6.1E-05
etot  6  Y  N  6  M  -913.22989040707  2.7E-06    0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1517.83428613413
   (E)  Total one-electron terms..... -4258.17649210294
   (I)  Total two-electron terms.....  1827.11231556174
   (L)  Electronic energy............. -2431.06417654120  (E+I)
   (N)  Total energy.................  -913.22989040707  (A+L)

 SCFE: SCF energy: HF    -913.22989040707 hartrees   iterations:   6
```

```
HOMO energy:    -0.29025
LUMO energy:     0.08211

 Orbital energies:
 -20.62903  -20.60347  -20.53834  -11.38042  -11.32743  -11.32384
 -11.30376  -11.27765  -11.26275  -11.26183  -11.25556  -11.25233
 -11.25140  -11.24516  -11.24475  -11.24462  -11.24422  -11.24369
 -11.24318  -11.24246  -11.23668   -1.48720   -1.43708   -1.37847
  -1.18793   -1.17042   -1.12261   -1.11316   -1.04568   -1.03522
  -1.02797   -1.02019   -0.93999   -0.89989   -0.87801   -0.86580
  -0.83898   -0.83296   -0.79399   -0.74615   -0.72956   -0.71458
  -0.69279   -0.68793   -0.67287   -0.66446   -0.66200   -0.64495
  -0.63864   -0.63398   -0.61839   -0.61326   -0.59829   -0.59487
  -0.59003   -0.58030   -0.55389   -0.54257   -0.52605   -0.51428
  -0.51232   -0.50909   -0.50311   -0.49347   -0.46699   -0.44190
  -0.44015   -0.38973   -0.34946   -0.34354   -0.32798   -0.29025
   0.08211    0.10025    0.12747    0.13205    0.16525    0.21080
   0.23131    0.24216    0.24945    0.27081

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    C10    -2.666313E-03  -2.943456E-04   9.687797E-04
  2    C1     -4.620870E-04   4.947788E-05  -8.814762E-04
  3    H2     -1.138376E-03  -1.785953E-04  -2.456291E-04
  4    C2     -4.273610E-04  -4.360119E-04  -3.196389E-04
  5    C3     -9.767572E-04  -1.524501E-04  -2.266979E-03
  6    C4     -1.796683E-03   1.394018E-05  -1.796802E-03
  7    C5      1.665287E-03   6.523094E-04   1.662316E-03
  8    C6      2.162356E-03   8.258715E-05   1.371011E-03
  9    C7      4.088610E-04  -1.533405E-04  -1.748975E-04
 10    C8     -1.458798E-04   1.389037E-04   2.387028E-04
 11    H6     -9.994164E-04  -2.652313E-05  -3.148777E-04
 12    H7     -1.193900E-03  -1.677799E-04   1.360224E-03
```

13	C9	1.951594E-03	1.659052E-04	4.881178E-04
14	O2	-1.482063E-03	-4.112601E-05	2.135258E-03
15	O1	5.756359E-04	2.655779E-04	-3.517902E-03
16	H13	1.194034E-03	1.281880E-04	4.554814E-04
17	O3	-7.193379E-05	-1.073073E-03	5.172984E-04
18	C11	1.686647E-03	6.483897E-04	-4.687102E-04
19	C13	-4.152813E-04	1.158247E-03	-1.575157E-03
20	C12	-2.049245E-03	1.619516E-03	1.306708E-03
21	H22	-3.071585E-04	2.239712E-05	-7.144054E-04
22	H23	-3.720273E-04	-4.824299E-04	4.044379E-04
23	H24	1.860155E-03	-6.027272E-04	-1.377370E-03
24	C14	1.188724E-03	-1.640832E-03	2.034265E-03
25	C15	2.665253E-04	2.835830E-03	-1.809252E-03
26	C16	3.099667E-03	-7.005223E-04	2.246551E-03
27	C17	-3.808992E-04	-1.989375E-03	1.204024E-03
28	C18	-2.585296E-03	-9.526530E-05	-2.210475E-03
29	H1	1.088499E-03	-3.530714E-04	1.503689E-03
30	H3	1.038459E-04	-1.513815E-03	5.043781E-04
31	H4	-7.142867E-04	2.842055E-05	-9.426287E-04
32	H5	-3.269897E-04	1.828456E-03	-7.397201E-04
33	H8	-9.519592E-04	-1.053415E-04	-6.889627E-04
total		-2.212080E-03	-3.684792E-04	-1.643642E-03

end of program der1b

start of program geopt 4

geometry optimization step 4
reading input hessian of dimension 99
in five columns format
reading input hessian of dimension 99
in five columns format
reading input hessian of dimension 99
in five columns format

Level shifts adjusted to satisfy step-size constraints
Step size: 0.3000039
Cos(theta): 0.2593765

Final level shift: -2.7058737E-03

energy change: -3.3037E-04 . (5.0000E-05)
gradient maximum: 4.7485E-03 . (4.5000E-04)
gradient rms: 1.1005E-03 . (3.0000E-04)
step size: 0.29990 trust radius: 0.30000

```
  displacement maximum:    1.3039E-01 .  (  1.8000E-03 )
  displacement rms:        2.6717E-02 .  (  1.2000E-03 )
  predicted energy change:    -6.0229E-04    geom step:   2.9990E-01
full step:   2.9990E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     8.2345E-03     y:    -3.0173E-02     z:    -9.6053E-03

  new geometry:
                                angstroms
  atom            x                y                z
  C10       0.4314598755     0.2164152238    -1.5155829466
  C1        0.7656884389     0.3147436896    -0.0772034677
  H2       -1.2023013887     0.0646042050     0.7066617209
  C2       -0.1603942795     0.2001224609     0.9438689988
  C3        2.5267311018     0.5592386806     1.5783793026
  C4        0.2248484840     0.2481958558     2.2803415001
  C5        2.1153731190     0.5228146033     0.2643992456
  C6        1.5747246655     0.4117703008     2.5743903440
  C7       -0.6902828589     0.1204472790     3.3953552486
  C8       -0.2374412064     0.1483991536     4.6472411463
  H6       -1.7440348143    -0.0011696227     3.1960653515
  H7       -0.8751940127     0.0512964961     5.5044767268
  C9        1.1943407296     0.3126769521     4.9213976650
  O2        1.6816706669     0.3346089773     6.0033583023
  O1        2.0116196033     0.4461097876     3.8478884788
  H13       3.5635834153     0.6985047966     1.8244840649
  O3        3.0588398519     0.6405209333    -0.6823207913
  C11       1.3461373038     0.5985159981    -2.3962456061
  C13      -0.8910603470    -0.3202609187    -1.9496858847
  C12       2.6737171414     1.1413116573    -1.9517990690
  H22       1.1589294851     0.5316042550    -3.4541381963
  H23       2.6591010916     2.2356678657    -1.9162892739
  H24       3.4645936942     0.8447324287    -2.6358748218
  C14      -3.3450956261    -1.3315447002    -2.7913146425
  C15      -1.3166631325    -1.5749457331    -1.5455613765
  C16      -1.7125120226     0.4179925144    -2.7770998228
  C17      -2.9303616331    -0.0851622596    -3.2000156790
  C18      -2.5336710517    -2.0769100120    -1.9586335144
  H1       -0.6875087243    -2.1564767527    -0.9140367667
  H3       -1.3999716498     1.3896606594    -3.0729264868
  H4       -3.5547627269     0.4940723173    -3.8326640360
  H5       -2.8521982896    -3.0478011785    -1.6320485399
  H8       -4.2953990957    -1.7253071704    -3.1071730584

  nuclear repulsion energy.......  1519.946723659 hartrees
  ------------------------------------------------
```

```
/  end of geometry optimization iteration   4   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.939E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       C10     C1     H2     C2     C3     C4     C5     C6
 grid # 1       92     88     71     86     89     89     82     86
 grid # 2      100     98    115     96     97     99     93     95
 grid # 3      192    198    209    183    183    198    181    185
 grid # 4      340    344    204    327    328    338    316    316

 number of gridpoints:
    atom        C7     C8     H6     H7     C9     O2     O1    H13
 grid # 1       86     88     73     73     79    111    108     73
 grid # 2       93     95    118    118     89    123    118    118
 grid # 3      186    185    218    224    169    270    248    224
 grid # 4      326    331    218    224    287    467    443    222

 number of gridpoints:
    atom        O3    C11    C13    C12    H22    H23    H24    C14
 grid # 1      111     87     90     77     72     70     70     89
 grid # 2      122     94    100     88    114    111    112     97
 grid # 3      250    183    194    158    219    222    219    183
 grid # 4      442    326    338    284    218    226    222    327

 number of gridpoints:
    atom       C15    C16    C17    C18     H1     H3     H4     H5
 grid # 1       86     85     89     89     71     71     73     73
 grid # 2       96     95     97     96    115    115    118    118
 grid # 3      182    182    183    184    218    216    222    222
 grid # 4      325    327    327    327    218    216    224    224

 number of gridpoints:
    atom        H8  total
```

```
 grid # 1       73   2750
 grid # 2      118   3471
 grid # 3      222   6712
 grid # 4      224   9826

 end of program grid


 start of program rwr
 end of program rwr


 start of program scf
```

	iter	updat	diis	incr	grid	total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	2	U	-913.19961700720		3.5E-04	1.3E-02
etot	2	Y	Y	6	M	-913.22543063497	2.6E-02	1.7E-04	4.9E-03
etot	3	N	Y	2	U	-913.22907178599	3.6E-03	5.3E-05	1.2E-03
etot	4	Y	Y	6	M	-913.22930720675	2.4E-04	1.8E-05	3.7E-04
etot	5	Y	Y	6	M	-913.22933323035	2.6E-05	7.5E-06	1.1E-04
etot	6	Y	Y	6	M	-913.22933418140	9.5E-07	3.3E-06	4.5E-05
etot	7	Y	N	6	M	-913.22933513183	9.5E-07	0.0E+00	0.0E+00

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1519.94672365898
   (E)  Total one-electron terms..... -4262.35559209320
   (I)  Total two-electron terms.....  1829.17953330238
   (L)  Electronic energy..... -2433.17605879082  (E+I)
   (N)  Total energy.............  -913.22933513183  (A+L)

 SCFE: SCF energy: HF    -913.22933513183 hartrees   iterations:   7


 HOMO energy:    -0.29084
 LUMO energy:     0.08099

  Orbital energies:
  -20.63163  -20.60347  -20.53907  -11.38240  -11.32919  -11.32294
  -11.30487  -11.27900  -11.26462  -11.26156  -11.25346  -11.25336
  -11.25182  -11.24722  -11.24364  -11.24139  -11.24044  -11.23983
  -11.23938  -11.23862  -11.23803   -1.48884   -1.43635   -1.37784
   -1.18888   -1.17355   -1.12325   -1.11341   -1.04419   -1.03730
   -1.02864   -1.02232   -0.93880   -0.90072   -0.87781   -0.86565
```

```
 -0.84303   -0.83333   -0.79313   -0.74707   -0.73070   -0.71658
 -0.69450   -0.68771   -0.67142   -0.66473   -0.66124   -0.64559
 -0.63982   -0.63496   -0.61899   -0.61390   -0.59836   -0.59520
 -0.59158   -0.58059   -0.55290   -0.54135   -0.52760   -0.51619
 -0.51310   -0.50921   -0.50308   -0.49453   -0.46697   -0.44237
 -0.43984   -0.39207   -0.34931   -0.34514   -0.32784   -0.29084
  0.08099    0.09798    0.12833    0.13369    0.16463    0.21127
  0.23405    0.24053    0.24960    0.26900

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    C10     7.491945E-04   2.981371E-04  -1.662035E-03
  2    C1     -1.688558E-03  -1.332012E-04   3.918768E-04
  3    H2      2.205587E-03  -1.281671E-04   2.239310E-04
  4    C2      1.129445E-03   8.287269E-04  -3.272710E-03
  5    C3      2.572247E-05  -1.419147E-04   3.003451E-03
  6    C4      1.470001E-03   7.194015E-05   2.208740E-04
  7    C5     -1.304834E-03  -6.963095E-04  -8.915723E-04
  8    C6      1.233269E-03   6.791833E-04  -2.779940E-03
  9    C7     -2.032858E-03  -3.090242E-04   1.192937E-03
 10    C8      6.480146E-06   1.532342E-04  -8.717990E-04
 11    H6      2.238462E-03   1.944633E-04  -9.182479E-05
 12    H7      1.116635E-03   2.727741E-04  -2.928073E-07
 13    C9      2.516040E-03  -5.040694E-04   8.058809E-03
 14    O2     -3.262053E-03   2.406118E-04  -5.078374E-03
 15    O1     -1.904064E-03  -2.101190E-04   6.018337E-04
 16    H13    -1.678070E-03  -2.217311E-04  -1.017336E-04
 17    O3     -1.592922E-03   1.136675E-03  -3.404548E-03
 18    C11    -4.990388E-04   2.983006E-04  -5.814389E-04
 19    C13     5.079954E-03   1.353255E-03   2.623008E-03
 20    C12     2.281104E-03   1.226016E-03  -4.575031E-04
 21    H22     5.836412E-04  -7.122448E-05   4.300844E-04
 22    H23     1.062297E-04  -3.487968E-03   7.317103E-04
```

```
  23    H24    -2.626889E-03   8.217733E-04   2.951678E-03
  24    C14    -5.368996E-03  -4.348754E-03  -2.080420E-04
  25    C15    -2.215190E-03  -3.111395E-03   3.281177E-04
  26    C16    -3.418080E-03  -2.615736E-04  -1.678627E-03
  27    C17     3.415330E-03   2.819110E-04   1.957479E-03
  28    C18     8.478666E-04  -3.756368E-03   2.100290E-03
  29    H1      4.426559E-03  -5.703125E-03   5.621484E-03
  30    H3      1.588596E-03   9.412692E-03  -4.033672E-03
  31    H4     -5.939692E-03   7.438145E-03  -7.124134E-03
  32    H5      2.683830E-04  -2.602285E-03   7.603190E-04
  33    H8      6.106425E-05   7.290735E-04  -6.176884E-04
 ----------   -------------  -------------  -------------
   total      -2.181680E-03  -2.503169E-04  -1.658052E-03

  end of program der1b


  start of program geopt   5

  geometry optimization step  5
  reading input hessian of dimension    99
   in five columns format
  reading input hessian of dimension    99
   in five columns format
  reading input hessian of dimension    99
   in five columns format
  ** restarting optimization from step    4 **


  energy change:           5.5528E-04 .  (  5.0000E-05 )
  gradient maximum:        4.7485E-03 .  (  4.5000E-04 )
  gradient rms:            1.1005E-03 .  (  3.0000E-04 )
  step size:   0.13676  trust radius:   0.30000
  displacement maximum:    6.6856E-02 .  (  1.8000E-03 )
  displacement rms:        1.2184E-02 .  (  1.2000E-03 )
  predicted energy change:    -3.3146E-04    geom step:   1.3676E-01
full step:   1.3676E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     2.2204E-16     y:    -8.3267E-17     z:    -1.1102E-16

  new geometry:
                              angstroms
  atom            x                y                z
  C10       0.4463405221      0.1824979973     -1.5233657224
  C1        0.7777078916      0.2835849644     -0.0839597480
  H2       -1.1814158871     -0.0084465104      0.6922967100
```

```
 C2       -0.1466120280      0.1558951084      0.9337175161
 C3        2.5257752319      0.5717613868      1.5810719245
 C4        0.2302230208      0.2235042494      2.2730170460
 C5        2.1217227679      0.5120168971      0.2637825165
 C6        1.5729690631      0.4212261341      2.5734559976
 C7       -0.6866546274      0.0838490915      3.3859641518
 C8       -0.2458940827      0.1455017133      4.6400364387
 H6       -1.7316907680     -0.0734021019      3.1802476549
 H7       -0.8848726802      0.0453394693      5.4964845633
 C9        1.1755845171      0.3586537476      4.9230710779
 O2        1.6460582895      0.4324532860      6.0053075002
 O1        1.9975593483      0.4860106771      3.8502970530
 H13       3.5578056884      0.7314745903      1.8306521850
 O3        3.0710167668      0.6303782680     -0.6760739673
 C11       1.3652598092      0.5507623119     -2.4050683142
 C13      -0.8835526632     -0.3401766732     -1.9515949157
 C12       2.7011986426      1.0750035269     -1.9683952980
 H22       1.1791479329      0.4826985358     -3.4633293071
 H23       2.7199624484      2.1661891214     -1.9875069543
 H24       3.4835048890      0.7227404844     -2.6276672048
 C14      -3.3533080261     -1.3303370388     -2.7868050073
 C15      -1.2764734072     -1.6336767064     -1.6208152896
 C16      -1.7453091402      0.4501518418     -2.6982667570
 C17      -2.9731001615     -0.0428830566     -3.1154733938
 C18      -2.4996378187     -2.1258077991     -2.0391739814
 H1       -0.6185264653     -2.2562707801     -1.0354136265
 H3       -1.4572759140      1.4561184573     -2.9464275960
 H4       -3.6293744380      0.5828738143     -3.6975833601
 H5       -2.7859633160     -3.1297754037     -1.7828736180
 H8       -4.3058712426     -1.7123604585     -3.1096498782

 nuclear repulsion energy.......  1518.536565699 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   5   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.924E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe
```

```
start of program grid

number of gridpoints:
   atom       C10     C1      H2      C2      C3      C4      C5      C6
grid # 1       92     88      71      86      89      89      84      87
grid # 2      100     98     115      96      97      99      94      95
grid # 3      192    198     209     183     183     199     180     184
grid # 4      340    344     206     327     328     338     315     314

number of gridpoints:
   atom        C7      C8      H6      H7      C9      O2      O1     H13
grid # 1       86      88      73      73      79     111     108      73
grid # 2       93      95     118     118      89     123     118     118
grid # 3      186     185     219     224     169     270     248     224
grid # 4      326     333     218     224     284     467     443     222

number of gridpoints:
   atom        O3     C11     C13     C12     H22     H23     H24     C14
grid # 1      111      87      92      77      72      69      70      89
grid # 2      121      94     100      86     114     111     112      97
grid # 3      251     182     195     156     220     222     219     184
grid # 4      443     326     338     282     219     226     219     327

number of gridpoints:
   atom       C15     C16     C17     C18      H1      H3      H4      H5
grid # 1       88      87      89      89      72      72      73      73
grid # 2       96      95      97      96     115     115     118     118
grid # 3      182     183     183     184     219     218     222     222
grid # 4      325     326     327     327     219     218     224     224

number of gridpoints:
   atom        H8   total
grid # 1       73    2760
grid # 2      118    3469
grid # 3      223    6718
grid # 4      224    9823

end of program grid


start of program rwr
end of program rwr


start of program scf

     i  u  d  i  g
```

	t e r	p d t	i i s	c u t	r i d	total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	2	U	-913.21233515020		2.7E-04	1.0E-02
etot	2	Y	Y	6	M	-913.22774238271	1.5E-02	1.4E-04	4.1E-03
etot	3	N	Y	2	U	-913.23001401051	2.3E-03	4.0E-05	1.0E-03
etot	4	Y	Y	6	M	-913.23013859183	1.2E-04	1.4E-05	2.9E-04
etot	5	Y	Y	6	M	-913.23016232967	2.4E-05	5.5E-06	8.1E-05
etot	6	Y	Y	6	M	-913.23016640677	4.1E-06	2.4E-06	3.3E-05
etot	7	Y	N	6	M	-913.23016760854	1.2E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1518.53656569928	
(E)	Total one-electron terms.....	-4259.57976711183	
(I)	Total two-electron terms.....	1827.81303380401	
(L)	Electronic energy.....	-2431.76673330782	(E+I)
(N)	Total energy.....	-913.23016760854	(A+L)

SCFE: SCF energy: HF -913.23016760854 hartrees iterations: 7

HOMO energy: -0.29031
LUMO energy: 0.08199

Orbital energies:

-20.63023	-20.60336	-20.53929	-11.38128	-11.32815	-11.32314
-11.30372	-11.27778	-11.26350	-11.26156	-11.25410	-11.25260
-11.25228	-11.24583	-11.24418	-11.24391	-11.24377	-11.24288
-11.24253	-11.24157	-11.23717	-1.48780	-1.43679	-1.38033
-1.18792	-1.17124	-1.12250	-1.11305	-1.04469	-1.03605
-1.02682	-1.02116	-0.93917	-0.90011	-0.87750	-0.86537
-0.83985	-0.83251	-0.79325	-0.74632	-0.72950	-0.71485
-0.69334	-0.68750	-0.67172	-0.66472	-0.66159	-0.64444
-0.63870	-0.63436	-0.61842	-0.61344	-0.59657	-0.59485
-0.59095	-0.58039	-0.55354	-0.54190	-0.52693	-0.51486
-0.51235	-0.50931	-0.50257	-0.49403	-0.46702	-0.44201
-0.43962	-0.39028	-0.34885	-0.34462	-0.32808	-0.29031
0.08199	0.09971	0.12804	0.13255	0.16512	0.21022
0.23138	0.24158	0.24975	0.26998		

end of program scf

start of program der1a
end of program der1a

```
 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	C10	1.414142E-03	3.275239E-04	-9.726409E-04
2	C1	-2.479701E-04	-3.930093E-05	-2.250598E-04
3	H2	5.732971E-04	7.043996E-05	1.387959E-04
4	C2	2.384221E-04	2.296282E-04	-9.097495E-04
5	C3	3.230985E-04	-6.518223E-05	6.420687E-04
6	C4	5.844896E-04	-2.862788E-04	2.387157E-04
7	C5	-1.564946E-04	-1.209369E-04	2.287316E-04
8	C6	-1.504076E-05	4.969720E-04	-1.285823E-03
9	C7	-1.399861E-03	-1.660823E-04	-3.883853E-04
10	C8	-6.155897E-04	-3.879209E-04	-5.866838E-05
11	H6	1.601377E-04	1.238554E-04	-2.294932E-04
12	H7	7.576192E-04	1.636067E-04	-5.885078E-04
13	C9	-8.829993E-04	9.985999E-04	-1.619869E-04
14	O2	1.423392E-03	-2.309374E-04	2.142955E-03
15	O1	-5.227083E-04	-4.774842E-04	9.421783E-04
16	H13	-8.818482E-04	-8.913350E-05	-1.886268E-04
17	O3	-1.583478E-03	1.342431E-05	-1.984320E-03
18	C11	-1.436093E-03	-5.053452E-04	4.047447E-04
19	C13	6.668288E-04	2.372922E-04	7.786719E-04
20	C12	1.343244E-03	1.085327E-03	6.572775E-05
21	H22	2.240779E-04	1.213059E-04	5.905388E-04
22	H23	-2.708586E-04	-1.128716E-03	6.789586E-04
23	H24	8.624767E-05	3.325819E-04	1.343914E-04
24	C14	-1.392776E-03	-5.038826E-04	-9.780308E-04
25	C15	5.980933E-04	-2.809238E-03	1.919015E-03
26	C16	-9.109368E-04	1.285189E-03	-1.556755E-03
27	C17	-6.890534E-04	2.771986E-03	-1.834564E-03
28	C18	7.853213E-04	-1.407277E-03	1.172041E-03
29	H1	-1.010420E-03	8.772933E-04	-1.444412E-03
30	H3	-2.203526E-05	1.386042E-04	-1.833287E-04
31	H4	6.240815E-04	-5.419813E-04	9.298293E-04
32	H5	-1.163721E-04	-6.832204E-04	2.226913E-04
33	H8	1.328590E-04	-9.018640E-05	6.639515E-05
total		-2.219183E-03	-2.594740E-04	-1.693902E-03

```
 end of program der1b
```

```
  start of program geopt   6

  geometry optimization step  6
  reading input hessian of dimension    99
   in five columns format
  reading input hessian of dimension    99
   in five columns format
  reading input hessian of dimension    99
   in five columns format


  energy change:          -2.7720E-04 .  (  5.0000E-05 )
  gradient maximum:        2.5933E-03 .  (  4.5000E-04 )
  gradient rms:            7.5154E-04 .  (  3.0000E-04 )
  step size:   0.18681  trust radius:   0.30000
  displacement maximum:    1.0195E-01 .  (  1.8000E-03 )
  displacement rms:        1.6643E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.9690E-04    geom step:   1.8681E-01
full step:   1.8681E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.2355E-03     y:    -1.4843E-02     z:    -4.8925E-03

  new geometry:
                                angstroms
  atom           x                 y                 z
  C10       0.4538053720      0.1805697878     -1.5320012608
  C1        0.7811438465      0.2820346784     -0.0902589374
  H2       -1.1846856563      0.0355186690      0.6803148931
  C2       -0.1484452129      0.1799673579      0.9248357217
  C3        2.5317107109      0.5358999347      1.5810175008
  C4        0.2254600061      0.2473173609      2.2665303731
  C5        2.1287353212      0.4821172209      0.2624080052
  C6        1.5720787484      0.4141263248      2.5708509825
  C7       -0.7002277327      0.1409238328      3.3775602158
  C8       -0.2598357906      0.1958053042      4.6323737824
  H6       -1.7491068283      0.0154973174      3.1682665541
  H7       -0.9023946185      0.1198695658      5.4863484774
  C9        1.1696823430      0.3685690694      4.9228558907
  O2        1.6409593215      0.4233293861      6.0076014050
  O1        1.9927477950      0.4702928985      3.8497644986
  H13       3.5658188653      0.6709849318      1.8326124115
  O3        3.0752974901      0.5713839939     -0.6837557781
  C11       1.3731086424      0.5583226990     -2.4076817752
  C13      -0.8781266486     -0.3456623086     -1.9563580054
```

```
 C12       2.7005853902      1.0959333657     -1.9528098340
 H22       1.1949589483      0.4944288511     -3.4657247124
 H23       2.6872814652      2.1944126363     -1.9009624692
 H24       3.4929275971      0.8075822004     -2.6421293659
 C14      -3.3521745087     -1.3337717616     -2.7689404976
 C15      -1.2518695879     -1.6539751823     -1.6496010105
 C16      -1.7606035398      0.4604717337     -2.6700295696
 C17      -2.9916842531     -0.0309009046     -3.0738462393
 C18      -2.4774495507     -2.1456819677     -2.0554683354
 H1       -0.5750891631     -2.2852796088     -1.1066762927
 H3       -1.4870953241      1.4774951511     -2.8955352374
 H4       -3.6669165537      0.6062291756     -3.6150585655
 H5       -2.7485862782     -3.1607121042     -1.8216045775
 H8       -4.3072822743     -1.7163407254     -3.0795024812

 nuclear repulsion energy.......  1518.005760312 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   6   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.938E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       C10     C1     H2     C2     C3     C4     C5     C6
 grid # 1       92     88     71     86     89     90     82     87
 grid # 2      100     98    115     96     97    101     93     95
 grid # 3      192    198    209    183    183    200    181    184
 grid # 4      340    345    207    327    328    341    316    312

 number of gridpoints:
    atom        C7     C8     H6     H7     C9     O2     O1    H13
 grid # 1       86     88     73     73     79    111    108     73
 grid # 2       93     95    118    118     89    123    118    118
 grid # 3      186    185    218    224    169    270    248    224
 grid # 4      326    333    218    224    286    467    443    222
```

number of gridpoints:

atom	O3	C11	C13	C12	H22	H23	H24	C14
grid # 1	110	87	92	78	72	70	70	89
grid # 2	121	94	100	90	114	112	112	97
grid # 3	250	182	194	159	220	222	219	183
grid # 4	442	324	340	285	219	226	223	327

number of gridpoints:

atom	C15	C16	C17	C18	H1	H3	H4	H5
grid # 1	88	87	89	89	72	72	73	73
grid # 2	96	95	97	96	116	115	118	118
grid # 3	181	182	183	184	220	218	223	223
grid # 4	326	328	328	328	220	218	224	224

number of gridpoints:

atom	H8	total
grid # 1	73	2760
grid # 2	118	3476
grid # 3	223	6720
grid # 4	224	9841

end of program grid

start of program rwr
end of program rwr

start of program scf

	iter	updi	dist	iguid		total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	2	U	-913.22300266890		1.8E-04	4.6E-03
etot	2	Y	Y	6	M	-913.22909473653	6.1E-03	8.4E-05	1.9E-03
etot	3	N	Y	2	U	-913.22994340891	8.5E-04	2.4E-05	4.5E-04
etot	4	Y	Y	6	M	-913.22999535168	5.2E-05	9.7E-06	1.6E-04
etot	5	Y	Y	6	M	-913.23000606376	1.1E-05	3.6E-06	6.6E-05
etot	6	Y	N	6	M	-913.23000817267	2.1E-06	0.0E+00	0.0E+00

Energy components, in hartrees:
(A) Nuclear repulsion..... 1518.00576031219
(E) Total one-electron terms..... -4258.55420474497
(I) Total two-electron terms..... 1827.31843626012

```
  (L)  Electronic energy..... -2431.23576848485  (E+I)
  (N)  Total energy.................  -913.23000817267  (A+L)

SCFE: SCF energy: HF    -913.23000817267 hartrees   iterations:   6


HOMO energy:    -0.29151
LUMO energy:     0.08178

 Orbital energies:
 -20.63042  -20.60261  -20.53978  -11.38230  -11.32850  -11.32225
 -11.30608  -11.27806  -11.26349  -11.26146  -11.25502  -11.25292
 -11.25235  -11.24621  -11.24434  -11.24413  -11.24357  -11.24329
 -11.24268  -11.24212  -11.23764   -1.48783   -1.43442   -1.37975
  -1.18710   -1.17006   -1.12175   -1.11222   -1.04347   -1.03500
  -1.02760   -1.01991   -0.93779   -0.89956   -0.87714   -0.86517
  -0.83902   -0.83228   -0.79242   -0.74636   -0.72910   -0.71498
  -0.69337   -0.68630   -0.67020   -0.66466   -0.66027   -0.64480
  -0.63865   -0.63335   -0.61849   -0.61337   -0.59813   -0.59492
  -0.58979   -0.57981   -0.55266   -0.54088   -0.52751   -0.51412
  -0.51144   -0.50869   -0.50269   -0.49359   -0.46525   -0.44215
  -0.43812   -0.39061   -0.34942   -0.34401   -0.32777   -0.29151
   0.08178    0.09958    0.12738    0.13251    0.16468    0.20837
   0.23175    0.24173    0.25009    0.26980

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    C10    -5.331542E-04   5.858875E-05   1.311585E-03
  2    C1      1.986665E-04   6.615780E-05  -4.287215E-05
  3    H2     -1.461025E-04  -6.597557E-06   1.099318E-04
  4    C2      3.205350E-04   1.804487E-04   4.349896E-04
  5    C3     -1.292358E-04   6.401816E-05  -5.597349E-04
  6    C4      2.436353E-04  -4.994782E-05  -6.939369E-04
```

7	C5	-9.017545E-04	-6.934918E-04	-3.118845E-04
8	C6	-1.484472E-03	-3.407657E-04	-8.525669E-04
9	C7	1.514746E-04	-4.384608E-05	-7.132188E-04
10	C8	1.631725E-03	3.560060E-04	5.626692E-04
11	H6	4.188576E-04	-3.845654E-05	3.299320E-05
12	H7	-3.002207E-04	-1.372742E-05	5.006026E-04
13	C9	-2.962335E-03	-5.472858E-04	4.389062E-04
14	O2	-1.960298E-04	1.421567E-04	-1.510804E-03
15	O1	1.542531E-03	3.581227E-04	1.128511E-03
16	H13	-1.818036E-04	1.243359E-05	-2.667942E-05
17	O3	3.771098E-04	3.818772E-03	-6.947140E-03
18	C11	5.338431E-04	1.150299E-03	-4.572622E-04
19	C13	-2.841650E-04	8.724634E-04	-9.644399E-04
20	C12	2.543738E-03	1.514896E-03	1.786195E-03
21	H22	-3.188027E-04	-1.004927E-05	-7.419033E-04
22	H23	1.211813E-04	-6.800511E-03	7.744331E-04
23	H24	-3.234251E-03	8.901598E-04	4.970725E-03
24	C14	1.058424E-03	-3.142325E-04	7.967993E-04
25	C15	1.413175E-04	3.008216E-03	-1.604397E-03
26	C16	2.710325E-03	-3.012219E-04	1.688822E-03
27	C17	-7.671293E-04	-2.639081E-03	1.011187E-03
28	C18	-2.448302E-03	8.778844E-04	-2.082126E-03
29	H1	1.393657E-03	-9.351337E-04	1.500838E-03
30	H3	2.202222E-04	-1.165505E-03	1.711593E-04
31	H4	-7.454439E-04	5.857439E-05	-8.225174E-04
32	H5	-3.997972E-04	4.596860E-04	-2.005726E-04
33	H8	-7.364426E-04	-2.249937E-04	-3.681670E-04
total		-2.162199E-03	-2.359643E-04	-1.679875E-03

```
 end of program der1b


 start of program geopt   7

 geometry optimization step  7
 [ turning on trust-radius adjustment ]
 reading input hessian of dimension    99
  in five columns format
 reading input hessian of dimension    99
  in five columns format
 reading input hessian of dimension    99
  in five columns format
 ** restarting optimization from step    6 **


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.1509609
```

```
   Cos(theta):   0.3968794

   Final level shift:  -2.5200854E-03

  energy change:           1.5944E-04 .  (  5.0000E-05 )
  gradient maximum:        2.5933E-03 .  (  4.5000E-04 )
  gradient rms:            7.5154E-04 .  (  3.0000E-04 )
  step size:   0.15095  trust radius:   0.15000
  displacement maximum:    7.5726E-02 .  (  1.8000E-03 )
  displacement rms:        1.3448E-02 .  (  1.2000E-03 )
  predicted energy change:    -2.8142E-04    geom step:   1.5095E-01
full step:   1.5095E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.1102E-16     y:     2.7756E-17     z:     5.5511E-16

  new geometry:
                                 angstroms
  atom            x                 y                 z
  C10        0.4443046331      0.1865333039     -1.5332853511
  C1         0.7746674285      0.2822811305     -0.0924057310
  H2        -1.1847347214      0.0366970027      0.6887953583
  C2        -0.1467015355      0.1765153433      0.9266896857
  C3         2.5319387405      0.5271825684      1.5786588379
  C4         0.2334977172      0.2355898588      2.2697913959
  C5         2.1204925382      0.4849002937      0.2602428418
  C6         1.5802496198      0.3982185499      2.5728791972
  C7        -0.6891355301      0.1288743983      3.3833921025
  C8        -0.2443108001      0.1741961963      4.6395141439
  H6        -1.7385945998      0.0139942744      3.1719837341
  H7        -0.8819651251      0.0989739908      5.4979134332
  C9         1.1852933302      0.3369119039      4.9327436653
  O2         1.6670043603      0.3741763431      6.0174875742
  O1         2.0064309421      0.4405343146      3.8533131849
  H13        3.5661906566      0.6620728271      1.8254344578
  O3         3.0590693504      0.5973229186     -0.6909094129
  C11        1.3634945541      0.5708190065     -2.4080955928
  C13       -0.8827638858     -0.3462573379     -1.9617556604
  C12        2.6907249564      1.1029156902     -1.9505024309
  H22        1.1858906873      0.5135150163     -3.4675211739
  H23        2.6838165890      2.1858576559     -1.9022767907
  H24        3.4870375810      0.8116124605     -2.6187283647
  C14       -3.3551518114     -1.3508957803     -2.7854554399
  C15       -1.2743022032     -1.6382465217     -1.6167634790
  C16       -1.7451657466      0.4334136776     -2.7224853145
  C17       -2.9757919803     -0.0652555561     -3.1307725815
  C18       -2.4991356308     -2.1380900193     -2.0291362076
```

```
 H1       -0.6107502961     -2.2504649608     -1.0383217062
 H3       -1.4562426605      1.4361831511     -2.9813447087
 H4       -3.6356647427      0.5523437874     -3.7101430545
 H5       -2.7845685494     -3.1382152470     -1.7661538883
 H8       -4.3088197831     -1.7366604758     -3.1028245625

 nuclear repulsion energy.......  1517.708000015 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   7   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.925E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       C10     C1     H2     C2     C3     C4     C5     C6
 grid # 1       92     88     71     86     89     93     84     87
 grid # 2      100     99    115     96     97    101     94     95
 grid # 3      192    198    210    182    183    199    180    184
 grid # 4      340    347    207    327    328    341    315    310

 number of gridpoints:
    atom        C7     C8     H6     H7     C9     O2     O1    H13
 grid # 1       85     88     73     73     79    111    108     73
 grid # 2       93     95    118    118     89    123    118    118
 grid # 3      186    185    218    224    169    270    248    224
 grid # 4      326    333    218    223    284    467    443    222

 number of gridpoints:
    atom        O3    C11    C13    C12    H22    H23    H24    C14
 grid # 1      112     87     92     77     72     69     70     89
 grid # 2      122     94    100     86    114    111    112     97
 grid # 3      251    182    195    155    220    222    218    185
 grid # 4      441    326    338    280    219    221    218    327

 number of gridpoints:
```

```
   atom       C15    C16    C17    C18     H1     H3     H4     H5
 grid # 1      87     87     89     89     72     72     73     73
 grid # 2      96     95     97     96    115    115    118    118
 grid # 3     183    183    183    184    219    218    222    222
 grid # 4     327    328    327    327    219    218    224    224

 number of gridpoints:
   atom        H8  total
 grid # 1      73   2763
 grid # 2     118   3473
 grid # 3     223   6717
 grid # 4     224   9819

 end of program grid


 start of program rwr
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  2  U  -913.22575406774            1.4E-04  6.1E-03
etot  2  Y  Y  6  M  -913.22945465321  3.7E-03   6.6E-05  2.5E-03
etot  3  Y  Y  6  M  -913.23000998476  5.6E-04   1.8E-05  7.0E-04
etot  4  N  Y  2  U  -913.23003218507  2.2E-05   1.0E-05  2.6E-04
etot  5  Y  Y  6  M  -913.23004132081  9.1E-06   2.5E-06  5.3E-05
etot  6  Y  N  6  M  -913.23003934152 -2.0E-06   0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1517.70800001464
   (E)  Total one-electron terms..... -4257.91204962997
   (I)  Total two-electron terms.....  1826.97401027381
   (L)  Electronic energy............. -2430.93803935617  (E+I)
   (N)  Total energy.................  -913.23003934152  (A+L)

 SCFE: SCF energy: HF    -913.23003934152 hartrees   iterations:   6


 HOMO energy:    -0.29143
 LUMO energy:     0.08060
```

Orbital energies:

-20.63022	-20.60190	-20.54041	-11.38334	-11.32875	-11.32336
-11.30194	-11.27912	-11.26381	-11.26202	-11.25469	-11.25321
-11.25266	-11.24691	-11.24418	-11.24404	-11.24399	-11.24318
-11.24269	-11.24197	-11.23810	-1.48516	-1.43925	-1.37756
-1.18780	-1.17040	-1.12190	-1.11270	-1.04546	-1.03609
-1.02643	-1.02044	-0.93983	-0.89926	-0.87772	-0.86544
-0.84029	-0.83268	-0.79324	-0.74659	-0.73002	-0.71530
-0.69518	-0.68814	-0.67188	-0.66437	-0.66090	-0.64541
-0.63864	-0.63345	-0.61858	-0.61444	-0.59706	-0.59534
-0.59100	-0.58074	-0.55292	-0.54133	-0.52720	-0.51434
-0.51175	-0.50865	-0.50244	-0.49342	-0.46577	-0.44255
-0.43892	-0.39127	-0.34887	-0.34455	-0.32745	-0.29143
0.08060	0.09919	0.12747	0.13201	0.16410	0.20934
0.23231	0.24153	0.25110	0.26999		

end of program scf

start of program der1a
end of program der1a

start of program rwr
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	C10	8.775728E-04	2.203975E-04	-4.600382E-04
2	C1	7.877551E-04	1.532655E-04	1.007748E-03
3	H2	-5.102343E-04	-1.775211E-04	6.748722E-05
4	C2	-1.299756E-03	-1.386728E-05	3.883996E-03
5	C3	4.060361E-04	3.258048E-04	-2.839897E-03
6	C4	-1.021020E-03	1.161272E-04	-1.228206E-03
7	C5	6.558473E-04	5.187498E-04	-5.666126E-04
8	C6	-1.970557E-03	-9.631107E-04	1.516119E-03
9	C7	1.525280E-03	2.116777E-04	7.096074E-04
10	C8	5.667107E-04	7.933528E-04	9.452863E-04
11	H6	1.593762E-04	-3.196216E-04	8.133533E-04
12	H7	-9.243570E-04	-1.033934E-04	-3.465064E-04
13	C9	2.300048E-03	-1.616104E-03	1.973961E-03
14	O2	-4.376368E-03	4.420721E-04	-8.489506E-03
15	O1	1.647555E-05	7.327201E-04	6.855078E-04

```
 16    H13     6.501872E-04   1.710700E-04  -2.142074E-04
 17    O3      4.112429E-03  -3.059154E-03   5.958110E-03
 18    C11    -6.821085E-04  -4.596212E-05  -1.228071E-03
 19    C13    -6.258517E-04   2.289562E-05  -4.534701E-04
 20    C12    -2.155210E-03  -9.297570E-04  -1.025282E-03
 21    H22    -3.741566E-04  -3.178648E-04  -1.338225E-05
 22    H23    -8.121423E-04   4.472471E-03  -4.437661E-04
 23    H24     9.672208E-05  -8.805470E-04  -1.758613E-03
 24    C14    -7.805091E-05   5.765098E-04  -5.122047E-04
 25    C15    -2.647353E-03   4.816135E-04  -2.039473E-03
 26    C16    -1.644610E-03  -2.421962E-04  -2.248372E-04
 27    C17     2.156922E-03  -3.510845E-05   1.079339E-03
 28    C18     2.172196E-03   1.978517E-03  -4.329662E-06
 29    H1      1.094998E-03  -2.015654E-03   1.790305E-03
 30    H3     -3.323005E-04   3.464601E-04  -3.671390E-04
 31    H4     -7.830757E-04   1.137275E-03  -1.127084E-03
 32    H5     -1.890017E-04  -2.221591E-03   9.150814E-04
 33    H8      5.913895E-04   5.206792E-05   3.324581E-04
-----------   -------------  -------------  -------------
   total      -2.256208E-03  -1.884043E-04  -1.664266E-03

 end of program der1b


 start of program geopt   8

 geometry optimization step  8
 reading input hessian of dimension    99
  in five columns format
 reading input hessian of dimension    99
  in five columns format
 reading input hessian of dimension    99
  in five columns format
 ** restarting optimization from step    6 **


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0750340
  Cos(theta):   0.4739450

  Final level shift:  -1.0338524E-02

 energy change:           1.2827E-04 .  (  5.0000E-05 )
 gradient maximum:        2.5933E-03 .  (  4.5000E-04 )
 gradient rms:            7.5154E-04 .  (  3.0000E-04 )
 step size:   0.07503  trust radius:   0.07500
 displacement maximum:    3.8284E-02 .  (  1.8000E-03 )
 displacement rms:        6.6845E-03 .  (  1.2000E-03 )
```

```
  predicted energy change:    -1.7910E-04    geom step:   7.5033E-02
full step:   7.5033E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.1102E-16     y:     2.7756E-17     z:    -4.4409E-16

  new geometry:
                                angstroms
  atom            x                 y                 z
  C10        0.4503379428      0.1781520551     -1.5302998417
  C1         0.7798176575      0.2776421129     -0.0895482118
  H2        -1.1792922579      0.0060402957      0.6868905186
  C2        -0.1441229843      0.1611888192      0.9279617277
  C3         2.5286446926      0.5504674212      1.5809893064
  C4         0.2309848892      0.2281798828      2.2698363401
  C5         2.1237738100      0.4956493130      0.2617955258
  C6         1.5744377153      0.4118436160      2.5729684348
  C7        -0.6916526835      0.1062331672      3.3812975505
  C8        -0.2511887674      0.1647497985      4.6365661394
  H6        -1.7378456903     -0.0332833171      3.1713733544
  H7        -0.8903112620      0.0783324872      5.4923380748
  C9         1.1736123652      0.3570278803      4.9272392070
  O2         1.6491478337      0.4160828288      6.0104575617
  O1         1.9963359108      0.4701775471      3.8527956168
  H13        3.5604286747      0.7010371479      1.8304442079
  O3         3.0698389634      0.6110605727     -0.6822489444
  C11        1.3680770107      0.5549894606     -2.4083742576
  C13       -0.8810918912     -0.3469592077     -1.9563520098
  C12        2.7003515905      1.0851572080     -1.9628183455
  H22        1.1865359958      0.4919786497     -3.4664936780
  H23        2.7039289602      2.1761770892     -1.9488456478
  H24        3.4900594594      0.7625734677     -2.6303374319
  C14       -3.3548001154     -1.3365509949     -2.7811398231
  C15       -1.2691518664     -1.6451111187     -1.6294650542
  C16       -1.7488346729      0.4475145963     -2.6969233009
  C17       -2.9796851085     -0.0444619315     -3.1066822480
  C18       -2.4946913432     -2.1372970337     -2.0418649123
  H1        -0.6034034578     -2.2689720426     -1.0635959269
  H3        -1.4636409792      1.4559028884     -2.9400616681
  H4        -3.6433908740      0.5842102193     -3.6705579201
  H5        -2.7773996005     -3.1438632854     -1.7905639497
  H8        -4.3095057686     -1.7183202142     -3.0968220920

  nuclear repulsion energy.......  1517.922517147 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   8   /
 ------------------------------------------------
```

```
end of program geopt


start of program onee
smallest eigenvalue of S:    2.922E-04
number of canonical orbitals.....          373
end of program onee


start of program probe
end of program probe


start of program grid

number of gridpoints:
   atom       C10     C1     H2     C2     C3     C4     C5     C6
grid # 1       92     88     71     86     89     91     84     87
grid # 2      100     98    115     96     97    101     94     95
grid # 3      192    198    209    182    183    199    180    184
grid # 4      340    345    206    327    328    342    316    314

number of gridpoints:
   atom        C7     C8     H6     H7     C9     O2     O1    H13
grid # 1       85     88     73     73     79    111    108     73
grid # 2       93     95    118    118     89    123    118    118
grid # 3      186    185    218    224    169    270    248    224
grid # 4      326    333    218    224    284    467    443    222

number of gridpoints:
   atom        O3    C11    C13    C12    H22    H23    H24    C14
grid # 1      112     87     92     77     72     69     70     89
grid # 2      122     94    100     86    114    111    112     97
grid # 3      251    182    194    156    220    222    219    184
grid # 4      441    324    340    282    219    226    220    327

number of gridpoints:
   atom       C15    C16    C17    C18     H1     H3     H4     H5
grid # 1       88     87     89     89     72     72     73     73
grid # 2       96     95     97     96    115    115    118    118
grid # 3      182    183    183    184    219    218    222    222
grid # 4      327    328    327    327    219    218    224    224

number of gridpoints:
   atom        H8  total
grid # 1       73   2762
grid # 2      118   3472
```

```
  grid # 3      224   6716
  grid # 4      224   9832

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                        energy  density   DIIS
      r  t  s  t  d     total energy       change  change    error

etot  1  N  N  2  U  -913.22799575569                1.0E-04  2.7E-03
etot  2  Y  Y  6  M  -913.22997072783  2.0E-03  4.7E-05  1.0E-03
etot  3  Y  Y  6  M  -913.23023141548  2.6E-04  1.3E-05  2.6E-04
etot  4  N  Y  2  U  -913.23025919149  2.8E-05  7.2E-06  1.1E-04
etot  5  Y  Y  6  M  -913.23026115701  2.0E-06  2.2E-06  4.4E-05
etot  6  Y  N  6  M  -913.23026267373  1.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1517.92251714721
   (E)  Total one-electron terms..... -4258.35855683780
   (I)  Total two-electron terms.....  1827.20577701686
   (L)  Electronic energy............. -2431.15277982094  (E+I)
   (N)  Total energy.................  -913.23026267373  (A+L)

 SCFE: SCF energy: HF    -913.23026267373 hartrees   iterations:   6


 HOMO energy:    -0.29102
 LUMO energy:     0.08146

  Orbital energies:
  -20.62984  -20.60275  -20.53980  -11.38209  -11.32819  -11.32323
  -11.30384  -11.27828  -11.26342  -11.26187  -11.25482  -11.25255
  -11.25253  -11.24618  -11.24422  -11.24411  -11.24410  -11.24321
  -11.24276  -11.24200  -11.23749   -1.48658   -1.43677   -1.37900
   -1.18765   -1.17048   -1.12215   -1.11269   -1.04476   -1.03560
   -1.02707   -1.02048   -0.93914   -0.89954   -0.87763   -0.86539
   -0.83970   -0.83263   -0.79317   -0.74625   -0.72958   -0.71500
   -0.69378   -0.68750   -0.67148   -0.66450   -0.66111   -0.64500
   -0.63860   -0.63372   -0.61851   -0.61372   -0.59749   -0.59497
```

```
 -0.59052   -0.58032   -0.55315   -0.54164   -0.52705   -0.51441
 -0.51189   -0.50889   -0.50270   -0.49357   -0.46622   -0.44228
 -0.43921   -0.39060   -0.34902   -0.34434   -0.32775   -0.29102
  0.08146    0.09962    0.12760    0.13222    0.16468    0.20956
  0.23185    0.24173    0.25013    0.27013

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	C10	-3.311045E-04	1.283840E-05	3.067989E-04
2	C1	3.361741E-04	7.433416E-05	1.478857E-04
3	H2	-3.624497E-04	-6.336365E-05	-1.887175E-05
4	C2	-5.382842E-04	-4.243262E-06	1.343538E-03
5	C3	-1.303153E-04	1.001366E-04	-1.523019E-03
6	C4	-6.659826E-04	-1.363202E-04	-9.740373E-04
7	C5	6.639483E-04	3.842599E-04	1.859943E-04
8	C6	-6.157734E-04	-1.856755E-04	4.690567E-04
9	C7	6.352749E-04	6.773366E-05	-2.158022E-04
10	C8	4.530268E-04	4.174016E-04	6.627988E-04
11	H6	-1.924550E-04	-1.262823E-04	1.559457E-04
12	H7	-5.945872E-04	-5.610773E-05	1.533878E-04
13	C9	4.232423E-04	-6.102459E-04	2.724198E-04
14	O2	-1.535827E-03	1.081825E-04	-2.185200E-03
15	O1	4.563936E-04	2.857867E-04	-2.275825E-05
16	H13	3.500005E-04	7.329269E-05	-2.333917E-05
17	O3	6.038551E-04	-6.267393E-04	-2.847977E-04
18	C11	2.309818E-04	2.886081E-05	-3.618900E-04
19	C13	-1.021099E-04	3.516615E-04	-5.913027E-04
20	C12	1.462073E-04	8.657382E-04	5.462955E-04
21	H22	-2.591579E-04	-6.594807E-05	-2.823553E-04
22	H23	-2.859397E-04	-7.650329E-04	4.650469E-05
23	H24	-8.865813E-04	1.771787E-04	8.067025E-04
24	C14	1.345456E-04	-2.328025E-04	2.246862E-04
25	C15	-9.274053E-04	1.019490E-03	-1.314674E-03

```
  26    C16     2.588785E-04  -2.192506E-04   4.395792E-04
  27    C17     6.765923E-04  -6.520372E-04   8.199880E-04
  28    C18     2.721066E-05   5.449071E-04  -4.789037E-04
  29    H1      8.636674E-04  -1.048637E-03   1.151666E-03
  30    H3     -4.366449E-05  -1.647855E-04  -1.395363E-04
  31    H4     -7.387286E-04   6.497360E-04  -9.470882E-04
  32    H5     -1.666825E-04  -4.006759E-04   1.115550E-04
  33    H8     -1.136084E-04  -6.533279E-05  -1.118006E-04
 -----------   -------------  -------------  -------------
   total       -2.230658E-03  -2.619420E-04  -1.630573E-03

  end of program der1b


  start of program geopt   9

  geometry optimization step  9
  reading input hessian of dimension    99
   in five columns format
  reading input hessian of dimension    99
   in five columns format
  reading input hessian of dimension    99
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0375401
   Cos(theta):   0.6035706

   Final level shift:  -2.8247406E-02

  energy change:          -9.5065E-05 .  (  5.0000E-05 )
  gradient maximum:        2.5306E-03 .  (  4.5000E-04 )
  gradient rms:            5.1707E-04 .  (  3.0000E-04 )
  step size:   0.03754  trust radius:   0.03750
  displacement maximum:    1.4429E-02 .  (  1.8000E-03 )
  displacement rms:        3.3443E-03 .  (  1.2000E-03 )
  predicted energy change:    -8.5659E-05    geom step:   3.7540E-02
full step:   3.7540E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.1329E-03     y:    -2.3793E-03     z:    -1.3266E-03

  new geometry:
                                angstroms
  atom            x                y                z
  C10       0.4443151029      0.1848533742     -1.5259533501
```

```
 C1        0.7768331141      0.2782358730     -0.0857294024
 H2       -1.1853127926      0.0154373662      0.6925491226
 C2       -0.1481230985      0.1637605310      0.9322710879
 C3        2.5313554034      0.5392043649      1.5784401453
 C4        0.2310981249      0.2272189063      2.2713935063
 C5        2.1238162693      0.4894289834      0.2623993951
 C6        1.5771336046      0.4039522125      2.5717374619
 C7       -0.6890216900      0.1106893128      3.3852072559
 C8       -0.2466893919      0.1710632621      4.6394371482
 H6       -1.7370084137     -0.0248480001      3.1794634482
 H7       -0.8865549982      0.0894645634      5.4963673121
 C9        1.1790704916      0.3567868795      4.9234694171
 O2        1.6520174747      0.4211537870      6.0062291505
 O1        2.0028001781      0.4625263206      3.8494174080
 H13       3.5651710455      0.6841600909      1.8266183273
 O3        3.0683276199      0.6015859715     -0.6828231432
 C11       1.3616327993      0.5650230010     -2.4037323995
 C13      -0.8836666457     -0.3427497846     -1.9562917256
 C12       2.6937773223      1.0919691058     -1.9547158769
 H22       1.1778105283      0.5062948198     -3.4622788445
 H23       2.6969686690      2.1812843571     -1.9280395888
 H24       3.4807586060      0.7778294784     -2.6270211224
 C14      -3.3527817956     -1.3401982150     -2.7871184675
 C15      -1.2720975972     -1.6390208203     -1.6257115683
 C16      -1.7486661038      0.4458961116     -2.7027356971
 C17      -2.9769943749     -0.0498326708     -3.1165793817
 C18      -2.4950248926     -2.1352388353     -2.0415713533
 H1       -0.6099832340     -2.2589402241     -1.0446963341
 H3       -1.4628251901      1.4521693425     -2.9505863834
 H4       -3.6375023184      0.5744644529     -3.6938073861
 H5       -2.7787346020     -3.1400937141     -1.7851602377
 H8       -4.3053794109     -1.7244317597     -3.1073232256

 nuclear repulsion energy.......  1518.412061634 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   9   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.926E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
```

end of program probe

start of program grid

number of gridpoints:

atom	C10	C1	H2	C2	C3	C4	C5	C6
grid # 1	92	88	71	86	89	89	82	87
grid # 2	100	98	115	96	97	99	93	95
grid # 3	192	198	209	183	183	199	181	184
grid # 4	340	345	207	327	328	340	315	314

number of gridpoints:

atom	C7	C8	H6	H7	C9	O2	O1	H13
grid # 1	85	88	73	73	79	111	108	73
grid # 2	93	95	118	118	89	123	118	118
grid # 3	186	185	219	224	169	270	248	224
grid # 4	326	333	218	224	284	467	443	222

number of gridpoints:

atom	O3	C11	C13	C12	H22	H23	H24	C14
grid # 1	112	87	91	77	72	69	70	89
grid # 2	122	94	100	86	114	111	112	97
grid # 3	250	182	194	156	220	222	219	184
grid # 4	441	326	338	282	219	224	219	327

number of gridpoints:

atom	C15	C16	C17	C18	H1	H3	H4	H5
grid # 1	88	87	89	89	72	72	73	73
grid # 2	96	95	97	96	115	115	118	118
grid # 3	182	183	183	184	219	218	222	222
grid # 4	325	327	327	327	219	218	224	224

number of gridpoints:

atom	H8	total
grid # 1	73	2757
grid # 2	118	3469
grid # 3	223	6717
grid # 4	224	9824

end of program grid

start of program rwr
end of program rwr

start of program scf

```
      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  1  U  -913.22984389360           6.1E-05  1.1E-03
etot  2  Y  Y  4  M  -913.23015481245  3.1E-04   2.0E-05  3.9E-04
etot  3  Y  Y  4  M  -913.23019643134  4.2E-05   5.5E-06  1.2E-04
etot  4  Y  Y  4  M  -913.23019952004  3.1E-06   2.7E-06  4.5E-05
etot  5  Y  N  4  M  -913.23020226313  2.7E-06   0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1518.41206163446
   (E)  Total one-electron terms..... -4259.33564208577
   (I)  Total two-electron terms.....  1827.69337818817
   (L)  Electronic energy............. -2431.64226389759  (E+I)
   (N)  Total energy.................  -913.23020226313  (A+L)

 SCFE: SCF energy: HF    -913.23020226313 hartrees   iterations:   5


 HOMO energy:    -0.29083
 LUMO energy:     0.08167

  Orbital energies:
  -20.63035  -20.60280  -20.53950  -11.38171  -11.32840  -11.32280
  -11.30312  -11.27810  -11.26355  -11.26155  -11.25437  -11.25267
  -11.25264  -11.24610  -11.24398  -11.24388  -11.24379  -11.24300
  -11.24263  -11.24176  -11.23747   -1.48739   -1.43743   -1.37987
   -1.18779   -1.17075   -1.12220   -1.11291   -1.04448   -1.03602
   -1.02656   -1.02087   -0.93906   -0.89989   -0.87751   -0.86539
   -0.83975   -0.83243   -0.79293   -0.74658   -0.72960   -0.71499
   -0.69419   -0.68744   -0.67149   -0.66466   -0.66129   -0.64474
   -0.63877   -0.63376   -0.61855   -0.61364   -0.59674   -0.59508
   -0.59085   -0.58041   -0.55328   -0.54144   -0.52729   -0.51462
   -0.51196   -0.50903   -0.50233   -0.49393   -0.46630   -0.44216
   -0.43912   -0.39076   -0.34879   -0.34453   -0.32788   -0.29083
    0.08167    0.09949    0.12773    0.13247    0.16485    0.20979
    0.23170    0.24163    0.25046    0.26998

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	C10	7.893627E-04	1.738318E-05	-4.795691E-04
2	C1	-9.891981E-05	9.514207E-05	-1.785597E-04
3	H2	2.170261E-04	-7.708063E-05	-1.733574E-05
4	C2	2.151263E-04	1.966231E-04	-4.628615E-04
5	C3	1.136705E-04	8.570018E-05	8.819887E-04
6	C4	4.996209E-04	-8.296247E-05	6.973481E-04
7	C5	-8.620994E-04	-2.136050E-04	-6.626503E-04
8	C6	-5.696045E-04	1.252785E-04	-6.592924E-04
9	C7	-5.007362E-04	7.887170E-05	-3.755862E-05
10	C8	-3.149054E-04	-1.435025E-04	-3.457814E-04
11	H6	1.443198E-04	-5.685646E-05	-1.144567E-04
12	H7	2.677368E-04	5.445897E-05	-2.936210E-04
13	C9	-4.127734E-04	1.868205E-04	3.418795E-04
14	O2	4.001292E-04	-2.108708E-05	1.965969E-04
15	O1	-3.844603E-04	-1.406104E-04	5.832355E-04
16	H13	-3.615840E-04	1.905670E-05	-7.514200E-05
17	O3	1.117319E-04	-6.065693E-04	-3.170937E-04
18	C11	-5.131738E-04	-1.467344E-05	-1.449557E-04
19	C13	1.506194E-04	-1.626867E-04	6.711972E-04
20	C12	2.988268E-04	2.503370E-04	-2.112694E-04
21	H22	8.631335E-05	-5.977836E-05	1.479348E-04
22	H23	-3.716078E-04	2.483225E-04	2.014745E-04
23	H24	-1.494605E-04	3.764323E-05	-3.895866E-05
24	C14	-5.735581E-04	2.101926E-04	-7.218672E-04
25	C15	1.630419E-04	-1.328959E-03	1.000390E-03
26	C16	-8.973636E-04	3.322190E-04	-8.365044E-04
27	C17	-1.513318E-04	9.293124E-04	-8.141822E-04
28	C18	6.462099E-04	-1.721535E-04	5.379609E-04
29	H1	-5.679877E-04	3.005432E-04	-7.362391E-04
30	H3	-7.675088E-05	4.054183E-04	-2.425374E-04
31	H4	3.279025E-04	-2.465017E-04	4.466880E-04
32	H5	-8.358751E-06	-5.496518E-04	1.482894E-04
33	H8	1.315992E-04	-3.172845E-05	6.681412E-05
total		-2.251439E-03	-3.350834E-04	-1.468638E-03

```
 end of program der1b
```

```
  start of program geopt  10

  geometry optimization step 10
  reading input hessian of dimension    99
   in five columns format
  reading input hessian of dimension    99
   in five columns format
  reading input hessian of dimension    99
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0188105
   Cos(theta):   0.5265513

   Final level shift:  -3.3444606E-02

  energy change:           6.0411E-05 .  (  5.0000E-05 )
  gradient maximum:        1.3597E-03 .  (  4.5000E-04 )
  gradient rms:            3.4776E-04 .  (  3.0000E-04 )
  step size:   0.01881  trust radius:   0.01875
  displacement maximum:    9.8315E-03 .  (  1.8000E-03 )
  displacement rms:        1.6758E-03 .  (  1.2000E-03 )
  predicted energy change:    -2.5249E-05    geom step:   1.8810E-02
full step:   1.8810E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.1922E-04     y:    -9.5973E-04     z:    -5.3515E-04

  new geometry:
                                angstroms
  atom            x                y                z
  C10       0.4455349095      0.1842865758     -1.5275524880
  C1        0.7777639593      0.2770220285     -0.0871651293
  H2       -1.1834047244      0.0157099873      0.6913525395
  C2       -0.1465166923      0.1638168619      0.9310484885
  C3        2.5316501611      0.5361916452      1.5786860629
  C4        0.2317777582      0.2274656316      2.2709409842
  C5        2.1243541999      0.4860606186      0.2616172339
  C6        1.5770567439      0.4031952696      2.5717298761
  C7       -0.6895077825      0.1126562262      3.3839757942
  C8       -0.2480956295      0.1739350352      4.6384943498
  H6       -1.7367793372     -0.0228737510      3.1769732865
  H7       -0.8878857936      0.0937841270      5.4950812034
  C9        1.1773910473      0.3588433440      4.9245140375
```

```
 O2        1.6515536264      0.4236292744      6.0068773459
 O1        2.0015216381      0.4622236888      3.8503417984
 H13       3.5651759031      0.6802688454      1.8269489270
 O3        3.0690242188      0.5963729000     -0.6843532524
 C11       1.3620334802      0.5666822688     -2.4048982499
 C13      -0.8833323725     -0.3433190572     -1.9561187252
 C12       2.6932774953      1.0944216579     -1.9533667950
 H22       1.1792777955      0.5084982370     -3.4634345767
 H23       2.6927191068      2.1839188211     -1.9186103111
 H24       3.4808254025      0.7866319419     -2.6275496508
 C14      -3.3530309820     -1.3394636725     -2.7855736096
 C15      -1.2716145048     -1.6398457717     -1.6251555793
 C16      -1.7487689780      0.4460601370     -2.7023972889
 C17      -2.9774725451     -0.0491121988     -3.1151118781
 C18      -2.4949168839     -2.1352465058     -2.0403656269
 H1       -0.6088858498     -2.2601729078     -1.0474978685
 H3       -1.4628623093      1.4524709248     -2.9506246707
 H4       -3.6386989580      0.5756330808     -3.6889890793
 H5       -2.7786177655     -3.1403562563     -1.7834021827
 H8       -4.3061084117     -1.7235308341     -3.1039450328

 nuclear repulsion energy.......  1518.394684456 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  10   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.922E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       C10     C1      H2      C2      C3      C4      C5      C6
 grid # 1       92     88      71      86      89      91      83      87
 grid # 2      100     98     115      96      97     101      93      95
 grid # 3      192    198     209     182     183     199     180     184
 grid # 4      340    345     207     327     328     341     315     314
```

number of gridpoints:

atom	C7	C8	H6	H7	C9	O2	O1	H13
grid # 1	85	88	73	73	79	111	108	73
grid # 2	93	95	118	118	89	123	118	118
grid # 3	186	185	219	224	169	270	248	224
grid # 4	326	333	218	224	284	467	443	222

number of gridpoints:

atom	O3	C11	C13	C12	H22	H23	H24	C14
grid # 1	112	87	92	77	72	69	70	89
grid # 2	122	94	100	86	114	111	112	97
grid # 3	250	182	194	156	220	222	219	184
grid # 4	441	326	338	282	219	226	218	327

number of gridpoints:

atom	C15	C16	C17	C18	H1	H3	H4	H5
grid # 1	88	87	89	89	72	72	73	73
grid # 2	96	95	97	96	115	115	118	118
grid # 3	182	183	183	184	219	218	222	222
grid # 4	325	327	327	327	219	218	224	224

number of gridpoints:

atom	H8	total
grid # 1	73	2761
grid # 2	118	3471
grid # 3	223	6715
grid # 4	224	9826

end of program grid

start of program rwr
end of program rwr

start of program scf

	iter	updi	diis	iguid	total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	1 U	-913.23018643780		2.0E-05	3.8E-04
etot	2	Y	Y	4 M	-913.23022083438	3.4E-05	6.6E-06	1.0E-04
etot	3	Y	Y	4 M	-913.23022314933	2.3E-06	1.9E-06	3.0E-05
etot	4	Y	N	4 M	-913.23022343666	2.9E-07	0.0E+00	0.0E+00

```
Energy components, in hartrees:
  (A)  Nuclear repulsion.....  1518.39468445613
  (E)  Total one-electron terms..... -4259.30224209937
  (I)  Total two-electron terms.....  1827.67733420658
  (L)  Electronic energy..... -2431.62490789279  (E+I)
  (N)  Total energy.............  -913.23022343666  (A+L)

SCFE: SCF energy: HF    -913.23022343666 hartrees   iterations:   4


HOMO energy:    -0.29111
LUMO energy:     0.08150

 Orbital energies:
 -20.63025  -20.60268  -20.53956  -11.38180  -11.32837  -11.32271
 -11.30315  -11.27823  -11.26351  -11.26150  -11.25447  -11.25262
 -11.25258  -11.24616  -11.24402  -11.24387  -11.24376  -11.24301
 -11.24262  -11.24180  -11.23759   -1.48714   -1.43708   -1.37969
  -1.18781   -1.17068   -1.12226   -1.11285   -1.04451   -1.03587
  -1.02673   -1.02075   -0.93903   -0.89968   -0.87770   -0.86547
  -0.83972   -0.83249   -0.79286   -0.74657   -0.72967   -0.71507
  -0.69430   -0.68737   -0.67140   -0.66462   -0.66117   -0.64478
  -0.63874   -0.63368   -0.61856   -0.61370   -0.59696   -0.59513
  -0.59074   -0.58035   -0.55326   -0.54137   -0.52742   -0.51461
  -0.51188   -0.50901   -0.50239   -0.49387   -0.46612   -0.44226
  -0.43911   -0.39088   -0.34888   -0.34445   -0.32780   -0.29111
   0.08150    0.09948    0.12768    0.13244    0.16475    0.20979
   0.23177    0.24169    0.25055    0.27007

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    C10     8.620732E-05  -9.909690E-05  -1.369928E-04
```

2	C1	1.104263E-04	8.145467E-05	-1.371198E-04
3	H2	-6.372607E-05	-5.888338E-05	-5.658912E-05
4	C2	-2.173762E-04	1.025453E-04	1.749147E-04
5	C3	-1.125266E-04	9.017172E-05	4.314340E-05
6	C4	-4.834746E-05	-1.109020E-04	4.212078E-05
7	C5	3.547236E-05	-4.873171E-05	-1.011800E-04
8	C6	-1.798884E-04	1.068366E-04	3.057091E-05
9	C7	-2.748926E-05	6.344999E-05	-6.187222E-05
10	C8	-8.931453E-05	-5.818365E-05	-5.711735E-05
11	H6	-1.977823E-04	-6.005729E-05	-8.221561E-05
12	H7	-9.435839E-05	-2.718815E-06	-1.032852E-04
13	C9	1.910158E-04	1.025957E-04	-2.881088E-04
14	O2	-1.325339E-04	-2.577218E-05	-4.107165E-05
15	O1	1.631217E-05	-1.455941E-05	1.386390E-04
16	H13	-7.672195E-05	4.030813E-05	-3.074379E-05
17	O3	-1.078065E-04	-4.441720E-04	-2.023684E-04
18	C11	-1.504413E-04	-4.663721E-05	-7.268463E-05
19	C13	1.625932E-04	4.129850E-05	1.772447E-04
20	C12	1.251874E-04	3.878743E-04	1.701034E-04
21	H22	-8.704595E-06	-3.169355E-05	3.182269E-06
22	H23	-2.691163E-04	-3.601645E-05	7.977054E-05
23	H24	-4.142052E-05	5.279533E-05	-9.191851E-05
24	C14	-3.568834E-04	-1.506326E-04	-2.921091E-04
25	C15	-2.070766E-04	-4.658274E-04	2.118800E-04
26	C16	-4.113906E-04	1.650209E-04	-4.630083E-04
27	C17	1.481010E-04	4.191902E-04	-2.641428E-04
28	C18	3.343141E-04	-2.202632E-04	3.821882E-04
29	H1	-9.056193E-05	-1.332836E-04	-1.070369E-04
30	H3	-7.096161E-05	2.412745E-04	-1.519844E-04
31	H4	-1.164622E-04	1.606691E-04	-1.410977E-04
32	H5	-1.601895E-05	-2.795747E-04	2.319648E-06
33	H8	2.090398E-05	-3.771185E-05	-4.190444E-05
total		-1.856376E-03	-2.692329E-04	-1.468474E-03

end of program der1b

start of program geopt 11

geometry optimization step 11
reading input hessian of dimension 99
in five columns format
reading input hessian of dimension 99
in five columns format
reading input hessian of dimension 99
in five columns format

```
  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0382490
   Cos(theta):   0.4103016

   Final level shift:  -9.6667240E-03

  energy change:          -2.1174E-05 *  (  5.0000E-05 )
  gradient maximum:        7.5510E-04 .  (  4.5000E-04 )
  gradient rms:            1.7399E-04 *  (  3.0000E-04 )
  step size:   0.03825  trust radius:   0.03750
  displacement maximum:    2.1170E-02 .  (  1.8000E-03 )
  displacement rms:        3.4075E-03 .  (  1.2000E-03 )
  predicted energy change:    -2.2396E-05    geom step:   3.8249E-02
full step:   3.8249E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.1463E-03     y:    -2.5840E-03     z:    -4.1426E-04

  new geometry:
                                angstroms
  atom            x                y                z
  C10       0.4424522772      0.1841118067     -1.5264583494
  C1        0.7757181572      0.2758147774     -0.0860283730
  H2       -1.1852679037      0.0220399202      0.6958168375
  C2       -0.1476000167      0.1669038008      0.9337966672
  C3        2.5324767231      0.5298472575      1.5783163176
  C4        0.2327629805      0.2300800524      2.2734150831
  C5        2.1233800977      0.4796749275      0.2616940497
  C6        1.5787472832      0.4017010934      2.5726433684
  C7       -0.6877531046      0.1196758091      3.3875822047
  C8       -0.2440449595      0.1805498336      4.6414251025
  H6       -1.7357065196     -0.0126055800      3.1816286493
  H7       -0.8827142546      0.1036237874      5.4990352403
  C9        1.1824705630      0.3611258236      4.9258675466
  O2        1.6581519600      0.4245359554      6.0079518466
  O1        2.0057126545      0.4603962198      3.8507158568
  H13       3.5666845080      0.6707821149      1.8249851169
  O3        3.0667410307      0.5861187977     -0.6864335455
  C11       1.3582691610      0.5704284200     -2.4030100196
  C13      -0.8857928196     -0.3438989007     -1.9565242436
  C12       2.6875554000      1.1007935013     -1.9476796701
  H22       1.1764611603      0.5138463025     -3.4617219660
  H23       2.6788823186      2.1900617291     -1.8961834858
  H24       3.4767351453      0.8082613016     -2.6277912903
  C14      -3.3530221476     -1.3405483014     -2.7927601617
  C15      -1.2760808586     -1.6395212243     -1.6237091649
```

```
 C16      -1.7481740001      0.4442516734     -2.7081215325
 C17      -2.9754356353     -0.0510812354     -3.1246437402
 C18      -2.4981079702     -2.1351599875     -2.0423055684
 H1       -0.6156721715     -2.2592733851     -1.0437130963
 H3       -1.4612681597      1.4498634308     -2.9573682210
 H4       -3.6342442759      0.5728567631     -3.7020878731
 H5       -2.7829076257     -3.1395381583     -1.7846772958
 H8       -4.3049886453     -1.7247366750     -3.1139522193

 nuclear repulsion energy.......  1518.228367726 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  11   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.921E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       C10     C1     H2     C2     C3     C4     C5     C6
 grid # 1       92     88     71     86     89     91     83     87
 grid # 2      100     98    115     96     97    101     93     95
 grid # 3      192    198    209    182    183    198    181    184
 grid # 4      340    345    207    327    328    342    315    314

 number of gridpoints:
    atom        C7     C8     H6     H7     C9     O2     O1    H13
 grid # 1       85     88     73     73     79    111    108     73
 grid # 2       93     95    118    118     89    123    118    118
 grid # 3      186    185    219    224    169    270    248    224
 grid # 4      326    333    218    224    284    467    443    222

 number of gridpoints:
    atom        O3    C11    C13    C12    H22    H23    H24    C14
 grid # 1      112     87     92     77     72     69     70     89
 grid # 2      121     94    100     86    114    111    112     97
 grid # 3      250    182    194    156    220    222    219    184
```

```
 grid # 4      441    326    338    282    219    226    218    327

 number of gridpoints:
    atom       C15    C16    C17    C18     H1     H3     H4     H5
 grid # 1       88     87     89     89     72     72     73     73
 grid # 2       96     95     97     96    115    115    118    118
 grid # 3      182    183    183    184    219    218    222    222
 grid # 4      326    327    327    327    219    218    224    224

 number of gridpoints:
    atom        H8  total
 grid # 1       73   2761
 grid # 2      118   3470
 grid # 3      223   6715
 grid # 4      224   9828

 end of program grid


 start of program rwr
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  1  U  -913.23004124088             3.2E-05  8.1E-04
etot  2  Y  Y  4  M  -913.23023010213  1.9E-04    1.4E-05  2.3E-04
etot  3  Y  Y  4  M  -913.23025452000  2.4E-05    4.3E-06  4.8E-05
etot  4  Y  N  4  M  -913.23025593997  1.4E-06    0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1518.22836772643
   (E)  Total one-electron terms..... -4258.96906621940
   (I)  Total two-electron terms.....  1827.51044255300
   (L)  Electronic energy..... -2431.45862366640  (E+I)
   (N)  Total energy.............  -913.23025593997  (A+L)

 SCFE: SCF energy: HF    -913.23025593997 hartrees   iterations:   4


 HOMO energy:    -0.29139
 LUMO energy:     0.08132
```

```
 Orbital energies:
 -20.63019  -20.60243  -20.53981  -11.38188  -11.32837  -11.32249
 -11.30319  -11.27838  -11.26374  -11.26160  -11.25457  -11.25291
 -11.25278  -11.24630  -11.24401  -11.24381  -11.24370  -11.24308
 -11.24257  -11.24180  -11.23764   -1.48709   -1.43700   -1.37960
  -1.18780   -1.17064   -1.12226   -1.11279   -1.04435   -1.03588
  -1.02677   -1.02065   -0.93885   -0.89956   -0.87778   -0.86553
  -0.83974   -0.83244   -0.79272   -0.74666   -0.72973   -0.71518
  -0.69456   -0.68726   -0.67122   -0.66459   -0.66102   -0.64486
  -0.63879   -0.63352   -0.61861   -0.61372   -0.59706   -0.59517
  -0.59071   -0.58034   -0.55315   -0.54117   -0.52763   -0.51463
  -0.51173   -0.50898   -0.50237   -0.49391   -0.46591   -0.44236
  -0.43899   -0.39111   -0.34889   -0.34443   -0.32773   -0.29139
   0.08132    0.09925    0.12758    0.13243    0.16458    0.20967
   0.23186    0.24147    0.25070    0.26987

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    C10     7.105191E-05   6.355124E-05  -1.106630E-04
  2    C1      2.650515E-05  -4.232418E-06   9.857618E-05
  3    H2     -1.193926E-04  -5.604243E-05  -7.919346E-05
  4    C2     -9.757664E-05   6.855236E-06   1.673549E-04
  5    C3     -1.245626E-04   8.396636E-05  -2.150910E-04
  6    C4     -2.748560E-04  -3.130623E-05  -1.770247E-04
  7    C5      1.423330E-04   3.113274E-05  -6.288999E-05
  8    C6      6.755251E-05  -1.351886E-05   1.421630E-04
  9    C7      1.124298E-04   1.943110E-05   2.696937E-05
 10    C8     -1.646614E-04   3.939180E-05  -6.495755E-05
 11    H6     -1.457249E-04  -5.756427E-05   8.690313E-06
 12    H7     -1.617897E-04  -2.611056E-05  -6.363235E-05
 13    C9      3.916835E-04  -7.740330E-05   1.397958E-04
```

```
 14    O2     -4.085586E-04   3.464896E-05  -6.288475E-04
 15    O1     -1.972892E-04   5.203442E-05   9.606488E-06
 16    H13     4.210916E-05   4.491448E-05  -3.761633E-06
 17    O3     -3.835374E-05  -2.720882E-04  -2.047507E-04
 18    C11    -1.967812E-05  -9.318835E-06  -1.217529E-04
 19    C13     1.297424E-04  -1.439419E-05   1.766071E-04
 20    C12     2.325316E-04   3.725988E-04  -4.055474E-05
 21    H22    -5.853280E-05  -3.384557E-05  -1.969156E-05
 22    H23    -1.719592E-04  -3.160637E-04  -1.040304E-05
 23    H24    -4.493733E-04   1.377722E-04   3.248537E-04
 24    C14    -2.023353E-04  -5.992777E-06  -3.392522E-04
 25    C15    -2.982873E-04  -1.088399E-04  -9.892392E-05
 26    C16    -3.875618E-04  -5.928353E-05  -3.292616E-04
 27    C17     1.074735E-04   1.002605E-04   4.183304E-05
 28    C18     2.589039E-04   8.961431E-05   1.888325E-04
 29    H1      1.291197E-04  -2.886651E-04   1.310420E-04
 30    H3      4.325366E-05   4.063045E-04  -1.885338E-04
 31    H4     -1.388051E-04   1.483352E-04  -1.611509E-04
 32    H5     -1.006920E-04  -4.350721E-04   6.106154E-05
 33    H8     -5.458569E-05  -9.002996E-05  -2.893379E-05
-----------   -------------  -------------  -------------
   total      -1.859886E-03  -2.689599E-04  -1.431884E-03

 end of program der1b


 start of program geopt  12

 geometry optimization step 12
 reading input hessian of dimension    99
  in five columns format
 reading input hessian of dimension    99
  in five columns format
 reading input hessian of dimension    99
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0537355
  Cos(theta):   0.2695053

  Final level shift:  -7.6202697E-04

 energy change:          -3.2503E-05 *  (  5.0000E-05 )
 gradient maximum:        6.7050E-04 .  (  4.5000E-04 )
 gradient rms:            1.6031E-04 *  (  3.0000E-04 )
 step size:   0.05373  trust radius:   0.05303
 displacement maximum:    2.8487E-02 .  (  1.8000E-03 )
```

```
  displacement rms:        4.7871E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.4131E-05    geom step:   5.3735E-02
full step:   5.3735E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.1525E-03     y:    -3.1465E-03     z:    -1.6863E-03

  new geometry:
                              angstroms
  atom            x                y                z
  C10       0.4402894482     0.1855937817    -1.5257408488
  C1        0.7751387646     0.2725236220    -0.0851366853
  H2       -1.1864973745     0.0273514083     0.6978719431
  C2       -0.1479184465     0.1677099917     0.9351181667
  C3        2.5348955310     0.5186239095     1.5773761025
  C4        0.2340507494     0.2302296948     2.2741430808
  C5        2.1242020473     0.4689328728     0.2615567986
  C6        1.5810528637     0.3966570393     2.5723393702
  C7       -0.6861871218     0.1258967480     3.3890849828
  C8       -0.2418985135     0.1896069115     4.6423505265
  H6       -1.7346452956    -0.0040466900     3.1843384969
  H7       -0.8806884261     0.1175430089     5.5003450802
  C9        1.1851001596     0.3666090859     4.9252886297
  O2        1.6608268000     0.4343959292     6.0067452495
  O1        2.0086967424     0.4574391624     3.8499651181
  H13       3.5699710500     0.6554126032     1.8232245802
  O3        3.0653590300     0.5693001350    -0.6896560347
  C11       1.3550205647     0.5780551385    -2.4009395093
  C13      -0.8872298634    -0.3432261714    -1.9566803123
  C12       2.6817028054     1.1095955406    -1.9389038579
  H22       1.1740662915     0.5254575821    -3.4599738414
  H23       2.6645028206     2.1969771749    -1.8641024927
  H24       3.4710907515     0.8362559204    -2.6251200909
  C14      -3.3530496801    -1.3414829994    -2.7965395188
  C15      -1.2788307653    -1.6380755580    -1.6214269245
  C16      -1.7477843419     0.4432568131    -2.7126786772
  C17      -2.9746965210    -0.0528029319    -3.1295404775
  C18      -2.5000226537    -2.1344727886    -2.0418089462
  H1       -0.6199731048    -2.2571412139    -1.0383867215
  H3       -1.4595527885     1.4485422051    -2.9647343775
  H4       -3.6323420025     0.5704546786    -3.7087020712
  H5       -2.7858242872    -3.1385870603    -1.7822310374
  H8       -4.3045301399    -1.7266566112    -3.1182936415

  nuclear repulsion energy.......  1518.380035455 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  12   /
```

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

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.920E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       C10     C1     H2     C2     C3     C4     C5     C6
 grid # 1       92     88     71     86     89     91     82     87
 grid # 2      100     98    115     96     97    101     93     95
 grid # 3      192    198    210    182    183    198    181    184
 grid # 4      340    345    207    327    328    341    316    314

 number of gridpoints:
    atom        C7     C8     H6     H7     C9     O2     O1    H13
 grid # 1       85     88     73     73     79    111    108     73
 grid # 2       93     95    118    118     89    123    118    118
 grid # 3      186    185    219    224    169    270    248    224
 grid # 4      326    333    218    224    284    467    443    222

 number of gridpoints:
    atom        O3    C11    C13    C12    H22    H23    H24    C14
 grid # 1      112     87     92     77     72     69     70     89
 grid # 2      121     94    100     85    114    111    112     97
 grid # 3      250    182    195    156    220    222    219    184
 grid # 4      441    326    338    282    219    226    218    327

 number of gridpoints:
    atom       C15    C16    C17    C18     H1     H3     H4     H5
 grid # 1       88     87     89     89     72     72     73     73
 grid # 2       96     95     97     96    115    115    118    118
 grid # 3      183    183    183    184    219    218    222    222
 grid # 4      326    327    327    327    219    218    224    224

 number of gridpoints:
    atom        H8  total
 grid # 1       73   2760
```

```
  grid # 2      118   3469
  grid # 3      224   6719
  grid # 4      224   9828

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  1  U  -913.22988307761           4.3E-05  1.1E-03
etot  2  Y  Y  4  M  -913.23022557035  3.4E-04   1.9E-05  3.4E-04
etot  3  Y  Y  4  M  -913.23026894554  4.3E-05   5.5E-06  7.1E-05
etot  4  Y  Y  4  M  -913.23026975462  8.1E-07   2.1E-06  2.8E-05
etot  5  Y  N  4  M  -913.23027253426  2.8E-06   0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1518.38003545499
   (E)  Total one-electron terms..... -4259.27355683059
   (I)  Total two-electron terms.....  1827.66324884134
   (L)  Electronic energy............. -2431.61030798925  (E+I)
   (N)  Total energy.................  -913.23027253426  (A+L)

 SCFE: SCF energy: HF    -913.23027253426 hartrees   iterations:   5


 HOMO energy:    -0.29170
 LUMO energy:     0.08122

  Orbital energies:
  -20.63032  -20.60222  -20.53976  -11.38188  -11.32844  -11.32232
  -11.30281  -11.27835  -11.26369  -11.26145  -11.25451  -11.25303
  -11.25277  -11.24637  -11.24401  -11.24385  -11.24345  -11.24308
  -11.24257  -11.24179  -11.23790   -1.48737   -1.43699   -1.37985
   -1.18781   -1.17056   -1.12226   -1.11282   -1.04421   -1.03593
   -1.02666   -1.02061   -0.93874   -0.89954   -0.87785   -0.86558
   -0.83966   -0.83234   -0.79246   -0.74693   -0.72979   -0.71525
   -0.69501   -0.68712   -0.67105   -0.66467   -0.66089   -0.64479
   -0.63887   -0.63329   -0.61867   -0.61382   -0.59694   -0.59531
```

```
  -0.59070   -0.58033   -0.55318   -0.54084   -0.52797   -0.51466
  -0.51164   -0.50896   -0.50214   -0.49403   -0.46556   -0.44241
  -0.43877   -0.39148   -0.34891   -0.34438   -0.32768   -0.29170
   0.08122    0.09906    0.12753    0.13245    0.16451    0.20967
   0.23189    0.24142    0.25109    0.26979

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  ------------  ------------
  1    C10     5.672385E-05  -3.087936E-05  -7.821212E-05
  2    C1      8.710413E-05  -8.398250E-06  -1.364661E-04
  3    H2     -7.235973E-05  -1.510193E-05  -3.928532E-05
  4    C2     -2.573747E-04   4.763035E-06   1.307452E-04
  5    C3     -2.581286E-05   1.802792E-05  -1.681632E-04
  6    C4     -1.462051E-04  -3.868582E-05  -6.011609E-05
  7    C5      3.563600E-05  -6.151633E-05  -9.146851E-05
  8    C6     -6.130733E-05   4.424807E-05   7.654231E-05
  9    C7     -6.527798E-05   8.216122E-06  -8.212042E-05
 10    C8     -2.567703E-04  -4.043680E-05  -8.238759E-06
 11    H6     -1.688701E-04  -1.856182E-05  -5.412747E-05
 12    H7     -1.017805E-04  -1.195846E-05  -6.175101E-05
 13    C9      2.679488E-04   3.490944E-05  -7.430515E-05
 14    O2     -1.073735E-04  -1.631822E-05   4.995366E-05
 15    O1     -1.653586E-04  -2.066796E-05  -7.189697E-05
 16    H13    -5.390706E-05   1.010743E-05  -2.535526E-05
 17    O3     -9.902401E-06   2.498916E-04  -2.152441E-04
 18    C11    -1.726762E-04   4.387774E-05  -5.326933E-05
 19    C13     2.402505E-05  -1.575735E-05  -2.603058E-05
 20    C12    -4.473446E-06  -2.194929E-04   1.710300E-04
 21    H22    -6.801397E-05  -1.084973E-05  -1.637266E-05
 22    H23    -6.569728E-05  -4.020767E-05   3.419042E-05
 23    H24     1.507990E-05   8.242854E-05  -1.252518E-04
 24    C14    -1.821625E-04  -3.283083E-04   7.612439E-05
```

25	C15	-2.763069E-04	-1.616361E-04	-3.245856E-05
26	C16	-1.729101E-04	1.521964E-04	-1.655187E-04
27	C17	2.747873E-04	3.331163E-04	-1.609215E-04
28	C18	1.792908E-04	-1.067704E-04	1.523634E-04
29	H1	1.973334E-05	-1.075436E-04	4.381919E-05
30	H3	-1.490948E-04	-9.802435E-05	-6.550222E-06
31	H4	-2.171847E-04	1.775670E-04	-3.038695E-04
32	H5	7.135620E-06	-9.407447E-05	-3.582860E-05
33	H8	6.773413E-06	6.650941E-06	-7.057450E-05
total		-1.826582E-03	-2.791893E-04	-1.428628E-03

end of program der1b

start of program geopt 13

geometry optimization step 13
reading input hessian of dimension 99
in five columns format
reading input hessian of dimension 99
in five columns format

energy change: -1.6594E-05 * (5.0000E-05)
gradient maximum: 5.0964E-04 . (4.5000E-04)
gradient rms: 1.0911E-04 * (3.0000E-04)
step size: 0.02665 trust radius: 0.10607
displacement maximum: 1.1524E-02 . (1.8000E-03)
displacement rms: 2.3741E-03 . (1.2000E-03)
predicted energy change: -4.9019E-06 geom step: 2.6649E-02
full step: 2.6649E-02
molecular structure not yet converged...

center of mass moved by:
x: 1.0458E-03 y: -2.6014E-03 z: -5.7192E-04

new geometry:

		angstroms	
atom	x	y	z
C10	0.4375123300	0.1885316910	-1.5245200489
C1	0.7740413901	0.2729789400	-0.0841207441
H2	-1.1887051608	0.0350245892	0.7004903086
C2	-0.1491547125	0.1712193202	0.9369106791
C3	2.5362235361	0.5128843530	1.5764040903
C4	0.2342957093	0.2319283157	2.2753380786
C5	2.1242343025	0.4651957569	0.2610370682
C6	1.5825897804	0.3934974082	2.5723303388

```
 C7       -0.6857361002      0.1317638562      3.3908445989
 C8       -0.2396837792      0.1932936013      4.6437067473
 H6       -1.7355521146      0.0067970763      3.1872514460
 H7       -0.8782837320      0.1241527955      5.5020617197
 C9        1.1892503531      0.3634379652      4.9253322771
 O2        1.6658655590      0.4282464166      6.0065911861
 O1        2.0117882190      0.4522107005      3.8495727351
 H13       3.5720213290      0.6468440235      1.8216097620
 O3        3.0637223119      0.5657623886     -0.6919314216
 C11       1.3509828771      0.5841229310     -2.3995389033
 C13      -0.8894755513     -0.3414262633     -1.9557927658
 C12       2.6767479261      1.1163193582     -1.9351262645
 H22       1.1697051204      0.5329945085     -3.4584797871
 H23       2.6542414250      2.2026249119     -1.8490635084
 H24       3.4662711933      0.8537018404     -2.6252521201
 C14      -3.3516504097     -1.3430696824     -2.8006340632
 C15      -1.2833739234     -1.6338518878     -1.6143462974
 C16      -1.7463327030      0.4410731098     -2.7199389716
 C17      -2.9709979410     -0.0565431200     -3.1403979175
 C18      -2.5028170397     -2.1319534450     -2.0366943138
 H1       -0.6271865834     -2.2501851304     -1.0251169156
 H3       -1.4570476992      1.4444654151     -2.9752522023
 H4       -3.6255424628      0.5634546505     -3.7273152358
 H5       -2.7901557154     -3.1345269796     -1.7722740135
 H8       -4.3017660304     -1.7296127566     -3.1245461969

 nuclear repulsion energy.......  1518.403055375 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  13   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.924E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       C10     C1      H2      C2      C3      C4      C5      C6
```

```
  grid # 1       92     88     71     86     89     90     82     87
  grid # 2      100     98    115     96     97     99     93     95
  grid # 3      192    198    210    183    183    200    182    184
  grid # 4      340    344    207    327    328    342    316    314

  number of gridpoints:
     atom        C7     C8     H6     H7     C9     O2     O1    H13
  grid # 1       86     88     73     73     79    111    108     73
  grid # 2       93     95    118    118     89    123    118    118
  grid # 3      186    185    219    224    169    270    248    224
  grid # 4      326    333    218    224    284    467    443    222

  number of gridpoints:
     atom        O3    C11    C13    C12    H22    H23    H24    C14
  grid # 1      111     87     92     77     72     69     70     89
  grid # 2      121     94    100     85    114    111    112     97
  grid # 3      250    182    195    156    220    222    219    184
  grid # 4      441    326    338    282    219    226    218    327

  number of gridpoints:
     atom       C15    C16    C17    C18     H1     H3     H4     H5
  grid # 1       88     87     89     89     72     72     73     73
  grid # 2       96     95     97     96    115    115    118    118
  grid # 3      183    183    183    184    219    218    223    223
  grid # 4      326    327    327    327    219    218    224    224

  number of gridpoints:
     atom        H8  total
  grid # 1       73   2759
  grid # 2      118   3467
  grid # 3      224   6725
  grid # 4      224   9828

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
       r  t  s  t  d     total energy   change  change    error

etot   1  N  N  1  U  -913.23006149363           3.3E-05  1.1E-03
```

```
etot   2  Y  Y  4  M  -913.23024927460  1.9E-04  1.5E-05  3.9E-04
etot   3  Y  Y  4  M  -913.23027667728  2.7E-05  4.7E-06  8.8E-05
etot   4  Y  N  4  M  -913.23027832940  1.7E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1518.40305537516
   (E)  Total one-electron terms..... -4259.31791919763
   (I)  Total two-electron terms.....  1827.68458549307
   (L)  Electronic energy............. -2431.63333370456  (E+I)
   (N)  Total energy.................  -913.23027832940  (A+L)

 SCFE: SCF energy: HF    -913.23027832940 hartrees   iterations:   4


 HOMO energy:    -0.29175
 LUMO energy:     0.08114

  Orbital energies:
 -20.63056  -20.60207  -20.53968  -11.38211  -11.32885  -11.32202
 -11.30259  -11.27854  -11.26381  -11.26127  -11.25443  -11.25333
 -11.25273  -11.24666  -11.24391  -11.24377  -11.24323  -11.24298
 -11.24253  -11.24181  -11.23813   -1.48767   -1.43704   -1.37993
  -1.18779   -1.17058   -1.12223   -1.11278   -1.04408   -1.03593
  -1.02671   -1.02057   -0.93860   -0.89964   -0.87780   -0.86558
  -0.83968   -0.83228   -0.79240   -0.74703   -0.72982   -0.71526
  -0.69521   -0.68709   -0.67101   -0.66474   -0.66092   -0.64476
  -0.63896   -0.63319   -0.61874   -0.61381   -0.59699   -0.59537
  -0.59068   -0.58029   -0.55307   -0.54067   -0.52807   -0.51475
  -0.51154   -0.50896   -0.50208   -0.49409   -0.46542   -0.44244
  -0.43873   -0.39168   -0.34894   -0.34437   -0.32759   -0.29175
   0.08114    0.09887    0.12743    0.13255    0.16446    0.20975
   0.23197    0.24131    0.25128    0.26967

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	C10	-2.346721E-04	-1.065659E-04	-1.161979E-06
2	C1	-1.870942E-04	-2.639211E-06	-7.934860E-05
3	H2	1.203775E-04	-1.141985E-05	-4.854501E-05
4	C2	-1.628691E-05	-6.215413E-07	-1.764828E-04
5	C3	-7.197567E-05	-2.391002E-05	1.992107E-04
6	C4	1.613373E-04	5.633450E-05	-4.424155E-05
7	C5	-2.688900E-04	5.714289E-05	-8.329275E-05
8	C6	-1.727915E-04	-5.017826E-05	-2.360705E-04
9	C7	-1.459396E-04	-3.293807E-05	1.997696E-04
10	C8	-3.401369E-05	-5.829828E-05	-1.190631E-04
11	H6	2.330182E-04	9.303886E-06	-2.547649E-05
12	H7	-2.375126E-05	-1.000416E-05	-1.273723E-05
13	C9	-5.451077E-04	8.612723E-05	2.420853E-04
14	O2	-1.169389E-04	-4.575087E-05	5.827893E-05
15	O1	-2.766466E-04	-7.225889E-05	-3.410677E-04
16	H13	-1.901199E-04	-9.821430E-06	-6.209110E-05
17	O3	6.278168E-05	6.590153E-05	1.655170E-05
18	C11	5.984350E-05	7.005549E-06	-7.596209E-05
19	C13	2.418658E-04	-2.046137E-05	7.823987E-05
20	C12	-1.697942E-04	-7.606498E-05	-1.048280E-04
21	H22	-3.961989E-05	6.686353E-06	-8.594606E-05
22	H23	2.363209E-05	1.211834E-04	-2.772397E-05
23	H24	1.399645E-05	3.296957E-06	-9.335379E-05
24	C14	-1.831072E-04	-2.576188E-04	3.965808E-06
25	C15	6.046187E-05	-2.760181E-04	1.362530E-04
26	C16	-1.424697E-04	-9.663690E-06	-9.929183E-05
27	C17	-1.817937E-04	3.317557E-05	-1.431146E-04
28	C18	-1.248507E-04	-1.561336E-04	-4.987816E-05
29	H1	-4.680559E-05	-7.843607E-06	-4.433838E-05
30	H3	4.855002E-05	4.135840E-04	-1.912623E-04
31	H4	-3.866240E-05	1.216914E-05	-6.410683E-05
32	H5	-1.024062E-05	4.174277E-05	-8.775474E-05
33	H8	-2.876452E-05	-2.659145E-05	-7.387541E-05
total		-2.224472E-03	-3.411483E-04	-1.436660E-03

```
 end of program der1b


 start of program geopt  14

 geometry optimization step 14
 reading input hessian of dimension    99
  in five columns format
 reading input hessian of dimension    99
```

```
   in five columns format
  reading input hessian of dimension    99
   in five columns format


  energy change:          -5.7951E-06 *  (  5.0000E-05 )
  gradient maximum:        4.6540E-04 .  (  4.5000E-04 )
  gradient rms:            1.3945E-04 *  (  3.0000E-04 )
  step size:   0.01595  trust radius:   0.05303
  displacement maximum:    8.0007E-03 .  (  1.8000E-03 )
  displacement rms:        1.4206E-03 .  (  1.2000E-03 )
  predicted energy change:    -3.4075E-06    geom step:   1.5947E-02
full step:   1.5947E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -6.0805E-04     y:     1.5073E-03     z:     3.4791E-04

  new geometry:
                              angstroms
  atom            x                y                z
  C10       0.4393464642     0.1867779493    -1.5254001045
  C1        0.7750961305     0.2727957796    -0.0850501330
  H2       -1.1869694285     0.0296107092     0.6985655712
  C2       -0.1481699499     0.1687643902     0.9355832274
  C3        2.5354234986     0.5171689213     1.5766807103
  C4        0.2342208631     0.2303022974     2.2743202371
  C5        2.1245396274     0.4683205868     0.2608624666
  C6        1.5816022782     0.3954060654     2.5720217140
  C7       -0.6858102307     0.1268051240     3.3895437074
  C8       -0.2411608856     0.1892442327     4.6427993639
  H6       -1.7346374150    -0.0016854319     3.1850601384
  H7       -0.8798343574     0.1176165197     5.5008997070
  C9        1.1865673428     0.3640696165     4.9252930068
  O2        1.6625877144     0.4299497698     6.0068366206
  O1        2.0094885795     0.4551042218     3.8496039748
  H13       3.5706613893     0.6534399588     1.8224372612
  O3        3.0651207008     0.5702572970    -0.6909832899
  C11       1.3533710855     0.5807248773    -2.4006789831
  C13      -0.8881055832    -0.3422721625    -1.9558475210
  C12       2.6796351181     1.1130864928    -1.9379239498
  H22       1.1721257032     0.5286438740    -3.4596700153
  H23       2.6594115390     2.2001049342    -1.8587042573
  H24       3.4695818193     0.8450036921    -2.6261592053
  C14      -3.3526300286    -1.3417056489    -2.7973082472
  C15      -1.2821617235    -1.6348759307    -1.6149169805
  C16      -1.7458249881     0.4416210350    -2.7179629533
  C17      -2.9717921988    -0.0549933013    -3.1365267072
```

```
 C18      -2.5027664007     -2.1318207714     -2.0358081644
 H1       -0.6253808017     -2.2520857419     -1.0272854983
 H3       -1.4562872634      1.4453433396     -2.9731632842
 H4       -3.6269797557      0.5660690399     -3.7215870194
 H5       -2.7901001313     -3.1344739649     -1.7723802327
 H8       -4.3035187764     -1.7272834185     -3.1200873690

 nuclear repulsion energy.......  1518.398683345 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  14   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.922E-04
 number of canonical orbitals.....          373
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       C10     C1     H2     C2     C3     C4     C5     C6
 grid # 1       92     88     71     86     89     91     82     87
 grid # 2      100     98    115     96     97    101     93     95
 grid # 3      192    198    210    183    183    199    181    184
 grid # 4      340    344    207    327    328    341    316    314

 number of gridpoints:
    atom        C7     C8     H6     H7     C9     O2     O1    H13
 grid # 1       85     88     73     73     79    111    108     73
 grid # 2       93     95    118    118     89    123    118    118
 grid # 3      186    185    219    224    169    270    248    224
 grid # 4      326    333    218    224    284    467    443    222

 number of gridpoints:
    atom        O3    C11    C13    C12    H22    H23    H24    C14
 grid # 1      111     87     92     77     72     69     70     89
 grid # 2      121     94    100     86    114    111    112     97
 grid # 3      250    182    195    156    220    222    219    184
 grid # 4      441    326    338    282    219    226    218    327
```

```
 number of gridpoints:
    atom       C15    C16    C17    C18     H1     H3     H4     H5
 grid # 1       88     87     89     89     72     72     73     73
 grid # 2       96     95     97     96    115    115    118    118
 grid # 3      183    183    183    184    219    218    223    223
 grid # 4      326    327    327    327    219    218    224    224

 number of gridpoints:
    atom        H8  total
 grid # 1       73   2759
 grid # 2      118   3470
 grid # 3      224   6723
 grid # 4      224   9827

 end of program grid


 start of program rwr
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  1  U  -913.23022395396             1.7E-05  3.8E-04
etot  2  Y  Y  4  M  -913.23027175927  4.8E-05  7.5E-06  1.4E-04
etot  3  Y  Y  4  M  -913.23027695089  5.2E-06  2.4E-06  3.4E-05
etot  4  Y  N  4  M  -913.23027900853  2.1E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1518.39868334525
   (E)  Total one-electron terms..... -4259.30795059134
   (I)  Total two-electron terms.....  1827.67898823755
   (L)  Electronic energy............. -2431.62896235378  (E+I)
   (N)  Total energy.................  -913.23027900853  (A+L)

 SCFE: SCF energy: HF    -913.23027900853 hartrees   iterations:   4


 HOMO energy:    -0.29171
 LUMO energy:     0.08118

 Orbital energies:
```

```
 -20.63043  -20.60233  -20.53987  -11.38198  -11.32848  -11.32240
 -11.30279  -11.27836  -11.26370  -11.26142  -11.25455  -11.25306
 -11.25285  -11.24646  -11.24397  -11.24389  -11.24341  -11.24307
 -11.24261  -11.24179  -11.23805   -1.48743   -1.43716   -1.37988
  -1.18782   -1.17055   -1.12225   -1.11279   -1.04417   -1.03590
  -1.02670   -1.02060   -0.93868   -0.89961   -0.87782   -0.86559
  -0.83967   -0.83232   -0.79248   -0.74696   -0.72982   -0.71523
  -0.69510   -0.68717   -0.67108   -0.66469   -0.66093   -0.64481
  -0.63887   -0.63322   -0.61869   -0.61382   -0.59700   -0.59536
  -0.59072   -0.58033   -0.55311   -0.54076   -0.52800   -0.51471
  -0.51160   -0.50895   -0.50212   -0.49406   -0.46558   -0.44245
  -0.43880   -0.39159   -0.34892   -0.34436   -0.32761   -0.29171
   0.08118    0.09890    0.12742    0.13247    0.16451    0.20975
   0.23193    0.24140    0.25110    0.26976

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    C10    -8.734011E-06   2.448429E-07  -5.133014E-05
  2    C1     -3.340506E-05   7.926606E-06   1.346035E-05
  3    H2     -4.906108E-05   1.752622E-05  -5.140438E-05
  4    C2     -3.002110E-05  -1.462056E-05  -1.597808E-04
  5    C3     -1.516700E-05  -1.518442E-05  -8.626329E-05
  6    C4     -6.029291E-05   8.137747E-06  -5.985064E-05
  7    C5     -1.326331E-04   3.454682E-05  -6.153216E-06
  8    C6     -3.143840E-05  -1.272514E-05  -6.447956E-05
  9    C7     -1.749137E-04  -1.786200E-05   2.863292E-05
 10    C8     -1.239769E-04  -1.678009E-06  -8.987203E-05
 11    H6     -7.556937E-05   2.114509E-05  -4.973643E-05
 12    H7     -1.001320E-04   6.950238E-06  -4.317043E-05
 13    C9     -5.878488E-05   8.216576E-06   2.434480E-04
 14    O2     -1.746193E-04  -3.445765E-05  -1.582139E-04
 15    O1     -1.818145E-04  -6.990530E-05  -7.297756E-05
 16    H13    -1.013658E-04  -1.520219E-05  -2.352424E-05
```

17	O3	-2.953309E-05	-1.574078E-04	1.636829E-04
18	C11	-6.382848E-05	-3.770103E-05	-6.568713E-05
19	C13	4.831142E-06	2.772571E-05	-8.853616E-05
20	C12	8.156342E-07	1.559643E-04	-2.197147E-04
21	H22	-4.989484E-05	9.033029E-06	-1.895745E-05
22	H23	-4.739341E-05	1.653294E-05	-7.590605E-05
23	H24	-2.108538E-04	4.685400E-05	7.875106E-05
24	C14	-9.111564E-05	-1.068476E-04	-4.957264E-05
25	C15	-7.585733E-05	-1.682412E-04	2.349501E-05
26	C16	-1.581509E-04	-4.377353E-05	-9.110815E-05
27	C17	5.121443E-05	1.157685E-04	-9.222480E-05
28	C18	7.586343E-06	-6.168535E-05	-3.392868E-05
29	H1	-5.625905E-05	-1.889178E-05	-1.037241E-05
30	H3	-2.173426E-05	1.224697E-04	-1.168030E-04
31	H4	-3.990781E-05	-2.096528E-05	-1.050303E-04
32	H5	-5.513207E-05	-8.924201E-05	-1.299140E-07
33	H8	-4.132210E-05	-6.299426E-05	-8.036918E-05
total		-2.228464E-03	-3.503427E-04	-1.413627E-03

 end of program der1b

 start of program geopt 15

 geometry optimization step 15
 reading input hessian of dimension   99
  in five columns format
 reading input hessian of dimension   99
  in five columns format
 reading input hessian of dimension   99
  in five columns format

 energy change: -6.7913E-07 # (5.0000E-05)
 gradient maximum: 3.0309E-04 * (4.5000E-04)
 gradient rms: 8.8500E-05 * (3.0000E-04)
 step size: 0.01029 trust radius: 0.05303
 displacement maximum: 3.9750E-03 . (1.8000E-03)
 displacement rms: 9.1678E-04 * (1.2000E-03)
 predicted energy change: -3.1820E-06   geom step: 1.0291E-02
full step: 1.0291E-02

 ****
 **   Geometry optimization complete   **
 ****

 center of mass moved by:

```
   x:     0.0000E+00     y:     0.0000E+00     z:     0.0000E+00

 final geometry:
                                angstroms
 atom           x                   y                   z
 C10       0.4393464642      0.1867779493     -1.5254001045
 C1        0.7750961305      0.2727957796     -0.0850501330
 H2       -1.1869694285      0.0296107092      0.6985655712
 C2       -0.1481699499      0.1687643902      0.9355832274
 C3        2.5354234986      0.5171689213      1.5766807103
 C4        0.2342208631      0.2303022974      2.2743202371
 C5        2.1245396274      0.4683205868      0.2608624666
 C6        1.5816022782      0.3954060654      2.5720217140
 C7       -0.6858102307      0.1268051240      3.3895437074
 C8       -0.2411608856      0.1892442327      4.6427993639
 H6       -1.7346374150     -0.0016854319      3.1850601384
 H7       -0.8798343574      0.1176165197      5.5008997070
 C9        1.1865673428      0.3640696165      4.9252930068
 O2        1.6625877144      0.4299497698      6.0068366206
 O1        2.0094885795      0.4551042218      3.8496039748
 H13       3.5706613893      0.6534399588      1.8224372612
 O3        3.0651207008      0.5702572970     -0.6909832899
 C11       1.3533710855      0.5807248773     -2.4006789831
 C13      -0.8881055832     -0.3422721625     -1.9558475210
 C12       2.6796351181      1.1130864928     -1.9379239498
 H22       1.1721257032      0.5286438740     -3.4596700153
 H23       2.6594115390      2.2001049342     -1.8587042573
 H24       3.4695818193      0.8450036921     -2.6261592053
 C14      -3.3526300286     -1.3417056489     -2.7973082472
 C15      -1.2821617235     -1.6348759307     -1.6149169805
 C16      -1.7458249881      0.4416210350     -2.7179629533
 C17      -2.9717921988     -0.0549933013     -3.1365267072
 C18      -2.5027664007     -2.1318207714     -2.0358081644
 H1       -0.6253808017     -2.2520857419     -1.0272854983
 H3       -1.4562872634      1.4453433396     -2.9731632842
 H4       -3.6269797557      0.5660690399     -3.7215870194
 H5       -2.7901001313     -3.1344739649     -1.7723802327
 H8       -4.3035187764     -1.7272834185     -3.1200873690

 nuclear repulsion energy.......  1518.398683345 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  15   /
------------------------------------------------

 end of program geopt


 start of program post
```

```
 Writing a SPARTAN archive file
 end of program post

Total cpu seconds     user:    1402.188   user+sys:    1402.188
```