```
+-----------------------------------------------------------------------
+
  |  Jaguar version 3.5, release  42
|
  |
|
  |  Copyright 1991-1998 Schrodinger, Inc.
|
  |  All Rights Reserved.
|
  |
|
  |  Use of this program should be acknowledged in publications as:
|
  |  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.
|
  +-----------------------------------------------------------------
--+

  start of program pre
  Job name: WF22859
  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
  H1       -1.2380580000      0.8466000000     -4.2883410000
  C1       -1.1728380000      0.8750760000     -3.1913210000
  H2       -2.4198140000      2.6176780000     -2.9570780000
  C2       -1.8210580000      1.8436700000     -2.4517330000
  C3       -0.2449540000     -0.1103290000     -1.1233040000
  C4       -1.7401660000      1.8468010000     -1.0483420000
  C5       -0.4084830000     -0.1064740000     -2.5236590000
  C6       -0.9617450000      0.8669150000     -0.3937330000
  C7       -2.4377370000      2.8262160000     -0.2546090000
  O3        0.1954790000     -1.0232580000     -3.3512560000
  C8       -2.3578500000      2.7847120000      1.0903200000
```

```
  H6       -3.0278950000      3.5942170000     -0.7795780000
  H7       -2.8644730000      3.5003580000      1.7532060000
  C9       -1.5720120000      1.7525730000      1.7468350000
  O2       -1.4009130000      1.5457370000      2.9463900000
  O1       -0.8770570000      0.8133610000      0.9774070000
  C11       0.6206920000     -2.2567580000     -2.7505380000
  C12       1.0399060000     -2.1414510000     -1.3362930000
  H14       1.4752090000     -2.5779450000     -3.4091330000
  H15      -0.2293180000     -2.9881360000     -2.8529390000
  C13       0.6392900000     -1.1199140000     -0.5501740000
  H17       1.6998130000     -2.9377830000     -0.9629500000
  C14       1.1355430000     -1.0193790000      0.8255080000
  C15       2.1714150000     -0.9029670000      3.4218160000
  C16       0.7517010000     -1.9689700000      1.7816690000
  C17       2.0437560000     -0.0122660000      1.1781390000
  C18       2.5591610000      0.0418980000      2.4719390000
  C19       1.2663890000     -1.9059310000      3.0754250000
  H20       0.0354050000     -2.7582370000      1.5106830000
  H21       2.3454450000      0.7375730000      0.4324310000
  H22       3.2692630000      0.8363240000      2.7441450000
  H23       0.9524090000     -2.6468700000      3.8250080000
  H24       2.5734950000     -0.8530420000      4.4440590000

  Molecular weight:    276.08 amu

  Stoichiometry:        C18H12O3
  Molecular Point Group: C1
  Point Group used: C1
  nuclear repulsion energy.......  1581.044227857 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:    3.023E-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        H1     C1     H2     C2     C3     C4     C5     C6
grid # 1       73     87     73     87     89     89     86     84
grid # 2      118     97    118     97     98     97     93     94
grid # 3      223    188    216    185    197    199    186    183
grid # 4      231    333    223    329    344    344    321    320

number of gridpoints:
   atom        C7     O3     C8     H6     H7     C9     O2     O1
grid # 1       86    110     85     73     73     83    111    109
grid # 2       93    120     94    118    118     93    123    119
grid # 3      187    252    187    216    224    170    269    247
grid # 4      331    443    333    223    233    298    471    437

number of gridpoints:
   atom       C11    C12    H14    H15    C13    H17    C14    C15
grid # 1       78     88     71     70     90     73     91     88
grid # 2       89     96    112    111     98    114     99     96
grid # 3      161    185    221    222    192    221    196    186
grid # 4      288    331    227    228    333    228    340    329

number of gridpoints:
   atom       C16    C17    C18    C19    H20    H21    H22    H23
grid # 1       87     88     88     88     73     72     73     73
grid # 2       95     96     96     96    115    117    118    118
grid # 3      184    185    185    185    219    221    223    223
grid # 4      328    330    329    329    227    228    231    231

number of gridpoints:
   atom       H24  total
grid # 1       73   2762
grid # 2      118   3474
grid # 3      223   6761
grid # 4      231   9982
```

```
 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  -910.20266796488                    5.4E-03  1.4E-01
etot  2  Y  Y  6  M  -912.86566990197  2.7E+00  2.0E-03  5.5E-02
etot  3  Y  Y  6  M  -913.11764117777  2.5E-01  8.3E-04  3.6E-02
etot  4  N  Y  2  U  -913.16155592894  4.4E-02  9.5E-04  2.0E-02
etot  5  Y  Y  6  M  -913.17563583693  1.4E-02  2.8E-03  1.6E-02
etot  6  N  Y  2  U  -913.19591241090  2.0E-02  2.7E-04  2.7E-03
etot  7  Y  Y  6  M  -913.19687654221  9.6E-04  1.1E-04  9.1E-04
etot  8  Y  Y  6  M  -913.19702451862  1.5E-04  2.7E-05  3.0E-04
etot  9  N  Y  2  U  -913.19681812930 -2.1E-04  1.1E-05  1.5E-04
etot 10  Y  Y  6  M  -913.19682675749  8.6E-06  6.7E-06  6.5E-05
etot 11  Y  Y  6  M  -913.19683395891  7.2E-06  2.2E-06  2.2E-05
etot 12  Y  N  6  M  -913.19682551284 -8.4E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1581.04422785738
   (E)  Total one-electron terms..... -4385.82836253504
   (I)  Total two-electron terms.....  1891.58730916481
   (L)  Electronic energy............. -2494.24105337022  (E+I)
   (N)  Total energy.................  -913.19682551284  (A+L)

 SCFE: SCF energy: HF    -913.19682551284 hartrees   iterations:  12
```

```
HOMO energy:    -0.29128
LUMO energy:     0.06631

 Orbital energies:
 -20.63073  -20.60577  -20.53494  -11.38783  -11.33988  -11.33176
 -11.30801  -11.29288  -11.27277  -11.26153  -11.26093  -11.25892
 -11.25821  -11.24744  -11.24505  -11.23651  -11.22857  -11.22797
 -11.22740  -11.22684  -11.22552   -1.46447   -1.41935   -1.34424
  -1.17883   -1.15462   -1.12109   -1.10097   -1.03695   -1.02682
  -1.00596   -1.00058   -0.92697   -0.88365   -0.87578   -0.86972
  -0.81383   -0.81116   -0.76847   -0.74041   -0.71964   -0.70518
  -0.68063   -0.67888   -0.66485   -0.65290   -0.64667   -0.63395
  -0.62144   -0.61762   -0.61083   -0.60160   -0.58949   -0.57589
  -0.57108   -0.55709   -0.54485   -0.53954   -0.52085   -0.51275
  -0.49692   -0.48725   -0.48390   -0.47733   -0.46770   -0.43699
  -0.43343   -0.39524   -0.32452   -0.32254   -0.31072   -0.29128
   0.06631    0.09847    0.14355    0.14984    0.15797    0.20820
   0.22248    0.24145    0.24558    0.25006

 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    H1      1.806584E-03  -7.317946E-04   1.878490E-02
  2    C1      1.656867E-03  -3.138027E-03  -4.091007E-03
  3    H2      9.626922E-03  -1.282355E-02   8.465703E-03
  4    C2     -2.929000E-04   1.255780E-04  -4.179390E-03
  5    C3     -1.595149E-02   1.616599E-02  -1.786570E-02
  6    C4      7.541916E-03  -1.000916E-02  -3.846039E-03
  7    C5     -3.162815E-04   1.093757E-03  -1.864941E-02
  8    C6      4.100902E-03  -6.341820E-03   1.916865E-03
  9    C7     -4.606629E-03   6.848241E-03   1.406718E-02
 10    O3     -6.246427E-03   1.058477E-02   3.863624E-02
```

11	C8	-1.035761E-02	1.434866E-02	-1.956470E-03
12	H6	9.161469E-03	-1.188665E-02	1.104328E-02
13	H7	9.193463E-03	-1.320003E-02	-1.141967E-02
14	C9	4.267450E-02	-5.532722E-02	7.803666E-02
15	O2	-2.546245E-02	3.279567E-02	-7.033859E-02
16	O1	-3.190849E-02	3.873125E-02	-3.706158E-02
17	C11	-5.801053E-03	-1.287595E-02	-3.817977E-02
18	C12	3.047214E-03	1.373460E-02	2.515233E-02
19	H14	-2.200874E-02	1.897355E-03	1.794709E-02
20	H15	1.936764E-02	1.192977E-02	-4.772737E-04
21	C13	1.217921E-02	-3.334573E-02	-2.296100E-02
22	H17	-9.294335E-03	1.472437E-02	-3.075714E-03
23	C14	1.207307E-02	-3.922908E-03	2.638032E-02
24	C15	1.536232E-03	-8.764535E-04	7.356893E-03
25	C16	-6.362521E-04	-1.653574E-03	-2.203594E-03
26	C17	1.279638E-03	1.579009E-03	-3.914293E-04
27	C18	4.113407E-03	6.171458E-03	-4.810205E-04
28	C19	-1.033811E-03	-4.192417E-03	5.959892E-03
29	H20	1.102096E-02	1.274689E-02	3.763489E-03
30	H21	-4.381069E-03	-1.162006E-02	1.099761E-02
31	H22	-1.069213E-02	-1.230989E-02	-4.175816E-03
32	H23	4.945883E-03	1.135459E-02	-1.144184E-02
33	H24	-6.210799E-03	-7.451526E-04	-1.574692E-02
total		1.254275E-04	-1.684026E-04	-3.376160E-05

```
 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:    0.3000091
  Cos(theta):   0.8989509

  Final level shift:  -9.5270018E-02

 gradient maximum:        7.7676E-02 .  (  4.5000E-04 )
 gradient rms:            1.4539E-02 .  (  3.0000E-04 )
 step size:   0.30000  trust radius:   0.30000
 displacement maximum:    1.0166E-01 .  (  1.8000E-03 )
 displacement rms:        2.7386E-02 .  (  1.2000E-03 )
```

```
  predicted energy change:    -2.5764E-02    geom step:   3.0000E-01
full step:   3.0000E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.3909E-02     y:     2.8039E-02     z:    -4.3526E-03

  new geometry:
                                angstroms
  atom            x                 y                 z
  H1       -1.2141069657      0.8125693367     -4.2762197061
  C1       -1.1662850139      0.8612704274     -3.2003804973
  H2       -2.4101254507      2.5752007042     -3.0018531145
  C2       -1.8221393239      1.8278267789     -2.4901585758
  C3       -0.2578785689     -0.0903221894     -1.1201381633
  C4       -1.7564485711      1.8471969005     -1.0949851857
  C5       -0.4114550982     -0.0975226774     -2.5130129061
  C6       -0.9807908661      0.8882793939     -0.4275351508
  C7       -2.4616196787      2.8215970771     -0.2956428643
  O3        0.1878699234     -1.0172272833     -3.2943680239
  C8       -2.3869277217      2.7995370078      1.0399741790
  H6       -3.0433142268      3.5761669154     -0.8090021828
  H7       -2.8973449866      3.4984425914      1.6807929235
  C9       -1.5870517396      1.7720121124      1.7368604866
  O2       -1.4733189148      1.7166407347      2.9144538206
  O1       -0.9269045107      0.8780554458      0.9281415886
  C11       0.5915840163     -2.2577183717     -2.7260920722
  C12       1.0157800383     -2.1221241478     -1.3054437822
  H14       1.4227720502     -2.6058631329     -3.3432367659
  H15      -0.2330033571     -2.9800117842     -2.8360983497
  C13       0.6308447271     -1.1155307114     -0.5261296307
  H17       1.6744415017     -2.8906418085     -0.9294370685
  C14       1.1712997927     -1.0403686117      0.8681549399
  C15       2.2421370798     -1.0025165263      3.4343406121
  C16       0.8351856274     -2.0235216633      1.7920070802
  C17       2.0557763260     -0.0371338888      1.2392047407
  C18       2.5869085628     -0.0178174429      2.5145700987
  C19       1.3668803791     -2.0042732122      3.0685329005
  H20       0.1530150069     -2.8032812581      1.5031445465
  H21       2.3223754226      0.7236144227      0.5291861918
  H22       3.2617239726      0.7643939485      2.8056529013
  H23       1.0989343356     -2.7659816030      3.7758484174
  H24       2.6540682209     -0.9805883991      4.4348747435

  nuclear repulsion energy.......  1580.920041035 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   1   /
 ------------------------------------------------
```

```
end of program geopt


start of program onee
smallest eigenvalue of S:    2.811E-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        H1     C1     H2     C2     C3     C4     C5     C6
grid # 1       73     85     73     87     89     89     86     86
grid # 2      118     95    118     97     97     98     93     94
grid # 3      223    183    216    182    196    199    182    184
grid # 4      222    325    216    327    341    344    317    311

number of gridpoints:
   atom        C7     O3     C8     H6     H7     C9     O2     O1
grid # 1       86    109     88     73     73     81    111    107
grid # 2       93    120     95    118    118     92    123    117
grid # 3      186    249    185    216    224    169    270    245
grid # 4      326    443    333    216    223    286    465    438

number of gridpoints:
   atom       C11    C12    H14    H15    C13    H17    C14    C15
grid # 1       79     87     70     72     92     72     92     88
grid # 2       88     94    112    112    100    114    100     96
grid # 3      158    182    218    222    193    218    195    182
grid # 4      284    326    225    226    335    218    341    327

number of gridpoints:
   atom       C16    C17    C18    C19    H20    H21    H22    H23
grid # 1       85     88     88     88     71     72     73     73
grid # 2       95     96     96     96    115    117    118    118
grid # 3      182    181    182    184    217    221    221    221
grid # 4      326    326    327    327    218    220    223    223

number of gridpoints:
   atom       H24  total
grid # 1       73   2759
grid # 2      118   3471
```

```
  grid # 3      221   6707
  grid # 4      223   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  -913.19714451728                 4.3E-04  1.2E-02
etot  2  Y  Y  6  M  -913.21690850629  2.0E-02        1.5E-04  3.4E-03
etot  3  N  Y  2  U  -913.21879793615  1.9E-03        5.3E-05  1.9E-03
etot  4  Y  Y  6  M  -913.21911005322  3.1E-04        2.3E-05  4.5E-04
etot  5  Y  Y  6  M  -913.21915803598  4.8E-05        8.7E-06  1.9E-04
etot  6  Y  Y  6  M  -913.21916633731  8.3E-06        3.7E-06  6.6E-05
etot  7  Y  N  6  M  -913.21916771155  1.4E-06        0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1580.92004103496
   (E)  Total one-electron terms..... -4385.31970153085
   (I)  Total two-electron terms.....  1891.18049278434
   (L)  Electronic energy..... -2494.13920874651  (E+I)
   (N)  Total energy.............  -913.21916771155  (A+L)

 SCFE: SCF energy: HF    -913.21916771155 hartrees   iterations:   7


 HOMO energy:    -0.29178
 LUMO energy:     0.07892

  Orbital energies:
  -20.62886  -20.60258  -20.54272  -11.38476  -11.33504  -11.32552
  -11.30303  -11.27733  -11.26343  -11.25891  -11.25742  -11.25278
  -11.24595  -11.23963  -11.23851  -11.23761  -11.22457  -11.22381
  -11.22331  -11.22286  -11.22191   -1.47752   -1.43135   -1.38050
   -1.18041   -1.15797   -1.11956   -1.10247   -1.03841   -1.03342
   -1.01025   -1.00700   -0.93192   -0.88771   -0.87880   -0.86738
   -0.82108   -0.81767   -0.77294   -0.74551   -0.72427   -0.70906
   -0.68881   -0.68316   -0.66969   -0.66038   -0.65587   -0.63573
```

```
 -0.62768   -0.61943   -0.61737   -0.61298   -0.59151   -0.58071
 -0.57701   -0.56221   -0.54786   -0.54417   -0.52129   -0.51867
 -0.50339   -0.49121   -0.48576   -0.48400   -0.46462   -0.43989
 -0.43502   -0.39565   -0.32984   -0.32617   -0.31177   -0.29178
  0.07892    0.10736    0.14574    0.15191    0.16301    0.21386
  0.23309    0.24600    0.25088    0.26036

 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	H1	6.039480E-04	-9.468670E-04	3.772338E-03
2	C1	4.536296E-03	-5.400989E-03	-1.047037E-03
3	H2	1.430833E-03	-2.093607E-03	1.628940E-03
4	C2	-1.335893E-03	2.014606E-03	3.673889E-03
5	C3	-4.727579E-03	4.072358E-03	-5.521863E-03
6	C4	4.889852E-03	-5.258620E-03	1.941078E-03
7	C5	-6.275980E-04	-1.080907E-03	-7.235977E-03
8	C6	-4.668017E-03	4.050898E-03	1.074246E-03
9	C7	-8.988775E-04	3.639659E-03	9.856974E-03
10	O3	2.184807E-03	-8.144043E-04	9.023198E-03
11	C8	-8.102939E-05	-4.554730E-03	-3.491407E-03
12	H6	1.641244E-03	-2.907535E-03	3.053729E-03
13	H7	1.896129E-03	-1.801778E-03	-2.701155E-03
14	C9	-3.508206E-04	9.927451E-03	-9.524174E-03
15	O2	3.143164E-03	-8.796632E-03	-8.434157E-03
16	O1	-6.815499E-03	7.015667E-03	4.294946E-03
17	C11	-5.733958E-03	-1.392234E-03	-1.056527E-02
18	C12	1.656639E-03	2.341453E-04	7.055075E-03
19	H14	-5.843555E-03	1.979576E-03	3.468710E-03
20	H15	5.692507E-03	5.305168E-03	7.793889E-04
21	C13	5.968172E-03	-7.449452E-03	-2.157948E-03
22	H17	-1.236342E-03	3.222992E-03	2.975558E-04
23	C14	-3.691256E-03	-3.247006E-03	8.865359E-04
24	C15	4.516410E-03	4.826897E-03	3.315007E-03

```
  25    C16    -6.663959E-04   4.429685E-05  -5.213254E-03
  26    C17    -3.847009E-04   1.055579E-04   9.566261E-04
  27    C18    -7.289141E-04  -2.195902E-03   4.028880E-03
  28    C19     6.714313E-04  -6.474664E-04   9.674686E-04
  29    H20    -6.265009E-04   1.933123E-04   4.623060E-04
  30    H21     7.282574E-04   1.500227E-03  -5.251887E-04
  31    H22     1.689104E-03   1.510206E-03  -5.127488E-04
  32    H23    -1.140346E-03  -1.556034E-03   7.455527E-04
  33    H24    -1.478172E-03   3.499046E-04  -4.542677E-03
 -----------   -------------  -------------  -------------
    total       2.133409E-04  -1.512389E-04  -1.904135E-04

  end of program der1b


  start of program geopt   2

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


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3007711
   Cos(theta):   0.4288783

   Final level shift:  -9.3393187E-03

  energy change:          -2.2342E-02 .  (  5.0000E-05 )
  gradient maximum:        2.1791E-02 .  (  4.5000E-04 )
  gradient rms:            4.2723E-03 .  (  3.0000E-04 )
  step size:   0.30073  trust radius:   0.30000
  displacement maximum:    1.0689E-01 .  (  1.8000E-03 )
  displacement rms:        2.7453E-02 .  (  1.2000E-03 )
  predicted energy change:    -3.4408E-03    geom step:   3.0073E-01
full step:   3.0073E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.4111E-02     y:    -3.5839E-02     z:    -6.7798E-03

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.0374420482      0.9251347601     -4.2752661067
  C1       -1.0357090813      0.9420894381     -3.2039163450
  H2       -2.2039996422      2.7051704494     -3.0018742997
  C2       -1.6843300570      1.9183345777     -2.4888717534
```

```
 C3       -0.2698679995     -0.0947004306     -1.1259320761
 C4       -1.6953274452      1.8925685034     -1.0942157621
 C5       -0.3578157868     -0.0679298196     -2.5209870539
 C6       -1.0052428040      0.8752254926     -0.4373683300
 C7       -2.3900762069      2.8640631727     -0.2728021103
 O3        0.2438395567     -1.0019784529     -3.2689762045
 C8       -2.3849567516      2.7744125583      1.0548052937
 H6       -2.9106474658      3.6652599436     -0.7625682742
 H7       -2.8793861761      3.4702181707      1.6987960266
 C9       -1.6805138381      1.6759320635      1.7181198003
 O2       -1.6540847206      1.4740343983      2.8708852823
 O1       -1.0462089806      0.7947920131      0.9044234075
 C11       0.5078494542     -2.2731590380     -2.7031690929
 C12       0.9505719770     -2.1617079261     -1.2763884830
 H14       1.2879566340     -2.7088298544     -3.3076398717
 H15      -0.3751251579     -2.8987898176     -2.8002658586
 C13       0.5948706713     -1.1442984778     -0.5097624725
 H17       1.5925139033     -2.9323524747     -0.8984930257
 C14       1.1523080600     -1.0371560493      0.8786080692
 C15       2.3156265069     -0.9070693930      3.4162046874
 C16       0.9110637905     -2.0390235785      1.8157330757
 C17       1.9806582984      0.0339643759      1.2259602964
 C18       2.5600544258      0.0979040976      2.4849109046
 C19       1.4908477730     -1.9744508585      3.0794633962
 H20       0.2622312331     -2.8643551262      1.5654625632
 H21       2.1783127657      0.8182258535      0.5050302256
 H22       3.2013446473      0.9309818203      2.7312150379
 H23       1.2892861606     -2.7589966581      3.7996720964
 H24       2.7553248001     -0.8572961921      4.3936071178

 nuclear repulsion energy.......  1584.850182734 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   2   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.828E-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        H1     C1     H2     C2     C3     C4     C5     C6
 grid # 1       73     87     73     87     89     89     85     85
 grid # 2      118     96    118     97    100     99     94     94
 grid # 3      223    183    218    183    196    198    182    181
 grid # 4      223    328    218    328    341    338    314    316

 number of gridpoints:
    atom        C7     O3     C8     H6     H7     C9     O2     O1
 grid # 1       85    111     87     73     73     80    111    107
 grid # 2       93    121     95    118    118     89    123    118
 grid # 3      184    249    185    218    224    166    268    245
 grid # 4      326    442    332    218    224    285    465    439

 number of gridpoints:
    atom       C11    C12    H14    H15    C13    H17    C14    C15
 grid # 1       77     87     70     69     92     72     91     88
 grid # 2       88     94    112    111    100    114    100     96
 grid # 3      156    182    218    222    194    218    196    184
 grid # 4      282    325    218    224    338    216    340    329

 number of gridpoints:
    atom       C16    C17    C18    C19    H20    H21    H22    H23
 grid # 1       87     88     88     88     71     72     73     73
 grid # 2       95     96     96     96    115    116    118    118
 grid # 3      183    184    184    183    218    220    222    222
 grid # 4      328    327    329    328    218    220    223    223

 number of gridpoints:
    atom       H24  total
 grid # 1       73   2754
 grid # 2      118   3474
 grid # 3      222   6711
 grid # 4      223   9828

 end of program grid


 start of program rwr
recomputing RwR matrix  16    grid:  4
 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	-913.16794508163		5.2E-04	1.6E-02
etot	2	Y	Y	6	M	-913.21462017931	4.7E-02	2.2E-04	6.4E-03
etot	3	N	Y	2	U	-913.22049349881	5.9E-03	6.0E-05	1.8E-03
etot	4	Y	Y	6	M	-913.22083356292	3.4E-04	2.8E-05	8.5E-04
etot	5	Y	Y	6	M	-913.22091871026	8.5E-05	1.0E-05	3.0E-04
etot	6	N	Y	2	U	-913.22092761525	8.9E-06	5.8E-06	8.9E-05
etot	7	Y	Y	6	M	-913.22092789672	2.8E-07	1.5E-06	3.6E-05
etot	8	Y	N	6	M	-913.22092626910	-1.6E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1584.85018273447	
(E)	Total one-electron terms.....	-4393.15465444646	
(I)	Total two-electron terms.....	1895.08354544289	
(L)	Electronic energy.....	-2498.07110900357	(E+I)
(N)	Total energy.....	-913.22092626910	(A+L)

SCFE: SCF energy: HF -913.22092626910 hartrees iterations: 8

HOMO energy: -0.29339
LUMO energy: 0.08024

Orbital energies:

-20.62537	-20.60168	-20.53823	-11.37832	-11.33124	-11.32288
-11.29955	-11.27692	-11.26301	-11.25756	-11.25416	-11.25146
-11.24433	-11.24010	-11.23717	-11.23628	-11.22707	-11.22690
-11.22590	-11.22552	-11.22393	-1.48841	-1.43580	-1.38532
-1.18030	-1.15482	-1.11997	-1.10320	-1.03947	-1.03453
-1.00750	-1.00593	-0.93382	-0.89144	-0.87873	-0.87001
-0.82113	-0.81648	-0.77336	-0.74940	-0.72483	-0.70830
-0.68889	-0.68792	-0.67130	-0.66332	-0.65968	-0.63690
-0.62870	-0.61960	-0.61718	-0.61154	-0.59236	-0.57720
-0.57666	-0.56330	-0.54967	-0.54530	-0.52180	-0.51778
-0.50257	-0.49095	-0.48592	-0.48238	-0.46212	-0.44069
-0.43310	-0.39738	-0.32922	-0.32603	-0.31060	-0.29339
0.08024	0.11007	0.14321	0.15054	0.16488	0.21682
0.23573	0.24611	0.25358	0.26269		

end of program scf

start of program der1a
end of program der1a

```
 start of program rwr
recomputing RwR matrix  16    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.253204E-04	1.077954E-04	-1.396560E-03
2	C1	3.326971E-04	-1.025843E-03	1.822797E-03
3	H2	-1.228198E-03	1.118500E-03	-1.166128E-03
4	C2	1.544407E-03	-1.202193E-03	1.118276E-03
5	C3	-3.761554E-04	-7.294388E-04	6.181464E-04
6	C4	1.330844E-03	-2.388458E-03	5.685321E-04
7	C5	1.308102E-04	-4.470938E-04	2.575978E-03
8	C6	2.397522E-04	8.200431E-05	-1.315701E-03
9	C7	4.982019E-04	-7.061806E-04	-2.439930E-04
10	O3	2.308910E-03	-2.722084E-04	-1.910451E-03
11	C8	2.886908E-03	-4.775221E-04	-1.202358E-03
12	H6	-1.305108E-03	1.485339E-03	-1.020481E-03
13	H7	-1.361135E-03	1.611843E-03	9.604414E-04
14	C9	-4.963740E-03	-3.373166E-04	-2.209067E-02
15	O2	1.041192E-03	-7.606475E-04	2.597638E-02
16	O1	3.804294E-03	-1.345328E-03	-2.717531E-03
17	C11	-1.489373E-03	3.554744E-03	3.199691E-03
18	C12	-5.167810E-04	-2.663594E-03	-2.411243E-03
19	H14	1.078396E-03	-7.407863E-05	-1.970386E-03
20	H15	-2.583887E-03	-2.425012E-04	-4.280432E-04
21	C13	-2.110932E-03	4.493369E-03	2.777224E-03
22	H17	2.457199E-03	-1.462552E-03	1.029149E-03
23	C14	6.877085E-04	1.946939E-03	1.734040E-03
24	C15	-3.780054E-03	-2.308566E-03	-4.942224E-03
25	C16	2.456757E-03	2.301305E-03	1.009636E-03
26	C17	-3.227425E-04	-1.011343E-03	2.182123E-05
27	C18	-1.924733E-03	-1.797059E-03	-2.430380E-03
28	C19	5.967313E-04	1.102939E-03	-2.991737E-05
29	H20	1.589491E-03	2.502792E-03	-1.694071E-05
30	H21	-1.333404E-03	-4.110250E-03	3.067549E-03
31	H22	-1.745407E-03	-2.626838E-03	3.826783E-04
32	H23	1.364995E-03	4.678548E-03	-3.482500E-03
33	H24	1.161356E-03	3.030958E-04	1.771247E-03
total		3.436821E-04	-6.997978E-04	-1.419205E-04

```
  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


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3007398
   Cos(theta):   0.2899022

   Final level shift:  -1.1449392E-02

  energy change:          -1.7586E-03 .  (  5.0000E-05 )
  gradient maximum:        2.5752E-02 .  (  4.5000E-04 )
  gradient rms:            3.2069E-03 .  (  3.0000E-04 )
  step size:   0.30073  trust radius:   0.30000
  displacement maximum:    2.1975E-01 .  (  1.8000E-03 )
  displacement rms:        2.7453E-02 .  (  1.2000E-03 )
  predicted energy change:    -2.0492E-03    geom step:   3.0073E-01
full step:   3.0073E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     8.5414E-03     y:    -1.1792E-02     z:     9.4049E-04

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.0278873309     0.9609018272    -4.2663319481
  C1       -1.0302153688     0.9602180735    -3.1931774587
  H2       -2.2668649663     2.6721407220    -2.9604380347
  C2       -1.7169279911     1.8996772408    -2.4593701820
  C3       -0.2459088602    -0.0814583869    -1.1327216873
  C4       -1.7301401338     1.8534909165    -1.0652960547
  C5       -0.3228218472    -0.0342735879    -2.5269596452
  C6       -1.0079139298     0.8555798903    -0.4271639549
  C7       -2.4603353366     2.7880791276    -0.2319324241
  O3        0.3154064456    -0.9357009813    -3.2852271092
  C8       -2.4551509710     2.6744322604     1.0920550698
  H6       -3.0098786911     3.5763657996    -0.7080131576
  H7       -2.9814591837     3.3385829934     1.7478827340
```

```
 C9       -1.7254367287      1.5937000182      1.7293197932
 O2       -1.7014851808      1.3450742319      2.8870906741
 O1       -1.0418246452      0.7564717941      0.9138610078
 C11       0.5406995011     -2.2185583145     -2.7279726178
 C12       1.0009216411     -2.1279155698     -1.3019013904
 H14       1.3012615971     -2.6711873662     -3.3454661321
 H15      -0.3708186945     -2.8122111572     -2.8211065973
 C13       0.6395097325     -1.1149707093     -0.5305050788
 H17       1.6607242041     -2.8933529411     -0.9368386276
 C14       1.1729278726     -0.9998207748      0.8593877465
 C15       2.3056080935     -0.8522152087      3.4047724924
 C16       0.7379072895     -1.8216942682      1.8537860486
 C17       2.1840279235     -0.1035366434      1.1505446122
 C18       2.7473598117     -0.0319608272      2.4130314417
 C19       1.3006489508     -1.7449432749      3.1231956857
 H20      -0.0547759112     -2.5074099493      1.6505744303
 H21       2.5454827872      0.5308925761      0.3802607519
 H22       3.5368223399      0.6597236599      2.6153665233
 H23       0.9383280143     -2.3777556185      3.8908228000
 H24       2.7369774974     -0.7942335086      4.3864466192

 nuclear repulsion energy.......  1590.533997889 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   3   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.791E-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        H1     C1     H2     C2     C3     C4     C5     C6
 grid # 1       73     87     73     87     90     93     86     84
 grid # 2      118     97    118     97    100    101     94     92
 grid # 3      223    183    218    183    198    197    183    183
 grid # 4      223    328    218    329    342    342    308    317
```

number of gridpoints:

atom	C7	O3	C8	H6	H7	C9	O2	O1
grid # 1	85	110	86	73	73	80	111	108
grid # 2	93	121	94	118	118	89	123	118
grid # 3	184	248	185	218	224	166	268	244
grid # 4	326	442	331	218	224	293	466	438

number of gridpoints:

atom	C11	C12	H14	H15	C13	H17	C14	C15
grid # 1	77	87	70	69	92	73	88	88
grid # 2	85	93	112	112	100	115	97	96
grid # 3	156	182	219	222	194	220	193	181
grid # 4	283	325	218	226	338	219	335	327

number of gridpoints:

atom	C16	C17	C18	C19	H20	H21	H22	H23
grid # 1	87	87	89	86	73	73	73	73
grid # 2	95	95	96	96	115	117	118	118
grid # 3	181	182	182	182	218	219	222	221
grid # 4	327	326	327	327	219	218	222	222

number of gridpoints:

atom	H24	total
grid # 1	73	2757
grid # 2	118	3469
grid # 3	222	6701
grid # 4	222	9826

end of program grid

start of program rwr
end of program rwr

start of program scf

	iter	updat	diis	incut	grid	total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	2	U	-913.11590598598		6.6E-04	3.4E-02
etot	2	Y	Y	6	M	-913.20413826957	8.8E-02	3.3E-04	1.4E-02
etot	3	N	Y	2	U	-913.21751049660	1.3E-02	1.0E-04	3.3E-03
etot	4	Y	Y	6	M	-913.21837470888	8.6E-04	3.6E-05	1.0E-03
etot	5	Y	Y	6	M	-913.21850743224	1.3E-04	1.4E-05	2.2E-04
etot	6	N	Y	2	U	-913.21850718150	-2.5E-07	5.3E-06	1.0E-04

```
etot   7  Y  Y  6  M  -913.21851195948  4.8E-06  2.2E-06  2.9E-05
etot   8  Y  N  6  M  -913.21851361671  1.7E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1590.53399788915
   (E)  Total one-electron terms..... -4404.50696418469
   (I)  Total two-electron terms.....  1900.75445267883
   (L)  Electronic energy............. -2503.75251150586  (E+I)
   (N)  Total energy.................  -913.21851361671  (A+L)

 SCFE: SCF energy: HF    -913.21851361671 hartrees   iterations:   8


 HOMO energy:    -0.29771
 LUMO energy:     0.07823

  Orbital energies:
 -20.62667  -20.60186  -20.53549  -11.37855  -11.33091  -11.32142
 -11.29976  -11.27890  -11.26378  -11.25598  -11.25375  -11.25224
 -11.24542  -11.23796  -11.23703  -11.23111  -11.21935  -11.21844
 -11.21812  -11.21709  -11.21585   -1.48855   -1.43644   -1.37578
  -1.18216   -1.16201   -1.12390   -1.10524   -1.04068   -1.03552
  -1.01560   -1.00535   -0.93455   -0.89241   -0.88033   -0.87233
  -0.82525   -0.81999   -0.77353   -0.75129   -0.72659   -0.71007
  -0.69167   -0.68897   -0.67152   -0.66243   -0.66002   -0.63639
  -0.62869   -0.62091   -0.61880   -0.61401   -0.59397   -0.58080
  -0.57443   -0.56408   -0.54957   -0.54460   -0.52163   -0.51888
  -0.50154   -0.49051   -0.48684   -0.48518   -0.46102   -0.44062
  -0.43146   -0.39677   -0.33009   -0.32423   -0.31444   -0.29771
   0.07823    0.10980    0.15048    0.15640    0.16353    0.21105
   0.23496    0.24902    0.25529    0.26219

 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	H1	-4.824711E-04	6.469609E-04	-1.111060E-04
2	C1	-2.662281E-03	3.455181E-03	1.148898E-03
3	H2	-1.527567E-03	1.826061E-03	-1.533281E-03
4	C2	2.121562E-03	-2.008832E-03	-1.644668E-03
5	C3	-4.753163E-04	-6.366800E-04	1.007659E-04
6	C4	-7.124686E-04	1.305026E-03	-3.133861E-03
7	C5	-1.230403E-04	-2.395440E-04	2.989020E-03
8	C6	3.348633E-03	-3.667896E-03	2.681825E-04
9	C7	8.084368E-04	-1.351403E-03	-2.584465E-03
10	O3	1.810489E-03	-1.546326E-03	1.434849E-03
11	C8	-2.088478E-03	5.680095E-03	5.887530E-04
12	H6	-1.558825E-03	2.110969E-03	-1.584297E-03
13	H7	-4.048644E-04	5.478671E-04	-1.248714E-04
14	C9	2.427074E-03	-1.456271E-02	8.836053E-03
15	O2	-2.341325E-03	7.535123E-03	1.991128E-03
16	O1	3.014891E-03	4.241701E-04	-6.734544E-03
17	C11	-1.676842E-03	7.599036E-04	1.275537E-03
18	C12	5.035784E-04	-2.724521E-04	-2.228027E-03
19	H14	3.525809E-04	-8.662427E-04	-1.334211E-03
20	H15	8.997056E-04	1.151454E-03	1.358064E-04
21	C13	-4.484309E-03	1.858192E-03	-8.269363E-04
22	H17	5.001169E-04	-4.668835E-04	5.705798E-04
23	C14	7.554200E-03	8.563859E-03	-1.259023E-02
24	C15	-3.243919E-03	-8.524901E-03	1.388731E-02
25	C16	-3.344635E-03	-1.072282E-02	2.059626E-02
26	C17	5.633744E-03	4.501730E-03	2.610533E-03
27	C18	5.691958E-03	1.226665E-02	-1.834160E-02
28	C19	-8.219022E-03	-4.631669E-03	-6.430604E-03
29	H20	-4.092563E-03	-5.451117E-03	1.491927E-03
30	H21	4.419970E-03	8.098930E-03	-8.258984E-03
31	H22	3.802521E-03	4.989790E-03	-1.714643E-03
32	H23	-5.288234E-03	-9.157668E-03	9.109338E-03
33	H24	-5.402507E-04	-1.308481E-03	1.894368E-03
total		-3.769532E-04	3.063350E-04	-2.470172E-04

```
 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
```

```
  ** restarting optimization from step    3 **


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3002851
   Cos(theta):   0.2145126

   Final level shift:  -3.6845431E-03

  energy change:           2.4127E-03 .  (  5.0000E-05 )
  gradient maximum:        2.5752E-02 .  (  4.5000E-04 )
  gradient rms:            3.2069E-03 .  (  3.0000E-04 )
  step size:   0.30021  trust radius:   0.30000
  displacement maximum:    1.2244E-01 .  (  1.8000E-03 )
  displacement rms:        2.7405E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.2974E-03    geom step:   3.0021E-01
full step:   3.0021E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     5.5511E-17     y:     2.2204E-16     z:    -1.8735E-16

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -0.9480909521     0.9893141385    -4.2689372148
  C1       -0.9716423691     0.9817132946    -3.1965187741
  H2       -2.1646071702     2.7245890498    -2.9837625171
  C2       -1.6468384589     1.9344588925    -2.4746237459
  C3       -0.2511127455    -0.0938317473    -1.1231370058
  C4       -1.6911578025     1.8734736781    -1.0802816532
  C5       -0.3041699189    -0.0355242835    -2.5181670152
  C6       -1.0089208325     0.8501381965    -0.4293512899
  C7       -2.4161808978     2.8189150041    -0.2501045347
  O3        0.3265239655    -0.9486551857    -3.2634712797
  C8       -2.4562649326     2.6837486344     1.0762358882
  H6       -2.9238756990     3.6347496403    -0.7306901342
  H7       -2.9796400683     3.3545769431     1.7249105320
  C9       -1.7873399846     1.5574156781     1.7295474727
  O2       -1.8451182159     1.3080961387     2.8921825030
  O1       -1.0844301627     0.7372035252     0.9098902428
  C11       0.4775740058    -2.2544153670    -2.7051238723
  C12       0.9538410767    -2.1669778615    -1.2821838314
  H14       1.2104339583    -2.7678770189    -3.3202431720
  H15      -0.4745815821    -2.7999968864    -2.7883525763
  C13       0.6143599898    -1.1459154894    -0.5130165738
  H17       1.6060119939    -2.9358758958    -0.9178931339
  C14       1.1817651467    -1.0245241408     0.8688450850
```

```
 C15       2.3409559676     -0.8530853691      3.3960593302
 C16       0.8370739653     -1.9338258896      1.8589640150
 C17       2.1187067165     -0.0273974390      1.1537903262
 C18       2.6965165370      0.0563253606      2.4065522171
 C19       1.4106626990     -1.8476161218      3.1191248205
 H20       0.1078476007     -2.7006039302      1.6550252667
 H21       2.4053383168      0.6773936216      0.3872889998
 H22       3.4237551512      0.8282060331      2.6085712984
 H23       1.1233367923     -2.5534202745      3.8817380760
 H24       2.7831945649     -0.7845578675      4.3715317082

 nuclear repulsion energy.......  1584.335486455 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   4   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.821E-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        H1     C1     H2     C2     C3     C4     C5     C6
 grid # 1       73     87     73     87     89     91     86     85
 grid # 2      118     97    118     97    100    101     94     94
 grid # 3      223    183    219    183    195    199    183    183
 grid # 4      223    328    218    329    338    341    310    315

 number of gridpoints:
    atom        C7     O3     C8     H6     H7     C9     O2     O1
 grid # 1       85    110     87     73     73     79    111    108
 grid # 2       93    120     95    118    118     89    123    117
 grid # 3      186    251    185    218    224    168    270    245
 grid # 4      326    443    331    218    224    285    465    438

 number of gridpoints:
    atom       C11    C12    H14    H15    C13    H17    C14    C15
 grid # 1       78     86     70     71     92     73     90     89
```

```
  grid # 2       88     94    112    112    100    114     98     96
  grid # 3      158    182    219    222    194    219    193    184
  grid # 4      284    326    222    226    338    219    340    327

  number of gridpoints:
     atom       C16    C17    C18    C19    H20    H21    H22    H23
  grid # 1       87     88     89     88     73     73     73     73
  grid # 2       95     96     96     96    114    117    118    118
  grid # 3      183    183    184    184    219    220    222    222
  grid # 4      328    327    327    328    219    220    223    223

  number of gridpoints:
     atom       H24  total
  grid # 1       73   2763
  grid # 2      118   3474
  grid # 3      223   6726
  grid # 4      223   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  -913.19038611192           3.7E-04  1.9E-02
etot   2  Y  Y  6  M  -913.21714162666  2.7E-02  1.7E-04  7.7E-03
etot   3  N  Y  2  U  -913.22094970832  3.8E-03  5.1E-05  2.0E-03
etot   4  Y  Y  6  M  -913.22119124204  2.4E-04  2.2E-05  7.0E-04
etot   5  Y  Y  6  M  -913.22124043958  4.9E-05  7.0E-06  1.5E-04
etot   6  Y  Y  6  M  -913.22124379650  3.4E-06  3.4E-06  4.1E-05
etot   7  Y  N  6  M  -913.22124336907 -4.3E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1584.33548645482
   (E)  Total one-electron terms..... -4392.12715195203
   (I)  Total two-electron terms.....  1894.57042212815
   (L)  Electronic energy............. -2497.55672982389  (E+I)
   (N)  Total energy.................  -913.22124336907  (A+L)
```

```
SCFE: SCF energy: HF    -913.22124336907 hartrees   iterations:   7


HOMO energy:    -0.29653
LUMO energy:     0.07894

 Orbital energies:
 -20.62847  -20.60197  -20.53834  -11.38209  -11.33208  -11.32157
 -11.30328  -11.27808  -11.26368  -11.25730  -11.25420  -11.25290
 -11.24524  -11.23928  -11.23816  -11.23679  -11.22657  -11.22571
 -11.22533  -11.22431  -11.22362   -1.48586   -1.43470   -1.37504
  -1.18127   -1.15635   -1.12015   -1.10293   -1.03757   -1.03630
  -1.00857   -1.00782   -0.93232   -0.89338   -0.87823   -0.86977
  -0.82140   -0.81795   -0.77262   -0.75092   -0.72499   -0.70905
  -0.68944   -0.68681   -0.67036   -0.66152   -0.65792   -0.63609
  -0.62802   -0.62001   -0.61649   -0.61259   -0.59233   -0.57892
  -0.57594   -0.56383   -0.54881   -0.54394   -0.52108   -0.51741
  -0.50090   -0.49018   -0.48663   -0.48367   -0.46093   -0.43994
  -0.43023   -0.39683   -0.32991   -0.32718   -0.31257   -0.29653
   0.07894    0.10953    0.14418    0.15073    0.16254    0.21154
   0.23561    0.24595    0.25371    0.26246

 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    H1     -2.772975E-05   6.205702E-05  -4.328442E-04
  2    C1     -6.161889E-04   6.674817E-04   1.222834E-03
  3    H2     -1.306407E-03   1.647831E-03  -7.302785E-04
  4    C2      1.342626E-03  -1.446369E-03   1.695028E-03
  5    C3      1.676580E-03  -3.029080E-03   6.936036E-04
  6    C4     -8.183604E-04   1.026407E-03   9.907076E-04
  7    C5     -1.134012E-04   1.104547E-03   2.768965E-03
  8    C6     -1.234749E-03   1.960494E-03  -1.869266E-04
  9    C7      1.109896E-03  -2.152508E-03   1.956157E-03
```

10	O3	3.207719E-03	-1.252129E-02	-5.697098E-04
11	C8	1.532432E-03	-3.216157E-04	-2.991912E-03
12	H6	-8.502843E-04	1.179651E-03	-5.931153E-04
13	H7	-1.197926E-03	1.413138E-03	4.322935E-04
14	C9	-5.219371E-03	-1.903791E-03	8.286050E-03
15	O2	4.012042E-03	2.504915E-03	-1.481729E-02
16	O1	2.926130E-03	-2.860228E-03	4.853415E-03
17	C11	-2.965388E-03	2.413644E-03	-1.023863E-04
18	C12	-1.717432E-03	-2.029133E-03	-3.986720E-03
19	H14	-2.964792E-03	3.896610E-03	5.134513E-05
20	H15	5.620051E-03	5.398415E-03	3.550397E-04
21	C13	-3.239393E-03	4.362705E-03	1.742648E-03
22	H17	1.675846E-03	-1.879296E-03	7.595609E-04
23	C14	2.464476E-03	3.653907E-03	-1.149328E-03
24	C15	-2.921020E-03	-2.343638E-03	-2.935792E-03
25	C16	2.524297E-04	2.425509E-04	3.854657E-04
26	C17	-2.746994E-03	-1.549958E-03	-3.177414E-03
27	C18	-2.546677E-04	-1.135554E-03	1.888545E-03
28	C19	3.103108E-03	3.166738E-03	1.237022E-03
29	H20	1.069451E-03	1.449712E-03	-5.668434E-04
30	H21	-1.736248E-03	-1.985682E-03	1.197198E-03
31	H22	-1.869874E-03	-2.141196E-03	2.250486E-04
32	H23	1.068935E-03	1.528263E-03	-7.015887E-04
33	H24	6.245773E-04	-1.529577E-04	1.846932E-03
total		-1.139269E-04	2.267663E-04	-3.542844E-04

```
 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


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3006625
  Cos(theta):   0.4955212

  Final level shift:  -1.7186224E-02

 energy change:          -3.1710E-04 .  (  5.0000E-05 )
 gradient maximum:        1.5155E-02 .  (  4.5000E-04 )
 gradient rms:            2.7232E-03 .  (  3.0000E-04 )
```

```
  step size:   0.30065  trust radius:   0.30000
  displacement maximum:    1.4861E-01 .  (  1.8000E-03 )
  displacement rms:        2.7445E-02 .  (  1.2000E-03 )
  predicted energy change:    -2.9989E-03    geom step:   3.0065E-01
full step:   3.0065E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     3.2154E-02     y:     3.0837E-02     z:    -2.5215E-03

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.0856066544     0.8721584901    -4.2654426195
  C1       -1.0764826572     0.8946635621    -3.1900552683
  H2       -2.2801782852     2.6431793654    -2.9916592984
  C2       -1.7329406119     1.8649467839    -2.4778333416
  C3       -0.2797925576    -0.1211621876    -1.1123812112
  C4       -1.7160171946     1.8549517019    -1.0852507914
  C5       -0.3764690613    -0.0984107488    -2.5049547388
  C6       -0.9973753350     0.8609252218    -0.4252957641
  C7       -2.4067347576     2.8419037052    -0.2828225849
  O3        0.2530178166    -1.0136636676    -3.2660389735
  C8       -2.3566926952     2.7970823769     1.0371642959
  H6       -2.9520928799     3.6266783271    -0.7835583049
  H7       -2.8526944074     3.5095020147     1.6728253501
  C9       -1.6239264666     1.7243867654     1.7012775303
  O2       -1.5104889100     1.6095660840     2.8461572286
  O1       -0.9706628485     0.8261643718     0.9146198397
  C11       0.4888352258    -2.2782411280    -2.6951131063
  C12       0.9534796827    -2.1796226106    -1.2787061625
  H14       1.2455971277    -2.7225884263    -3.3270332580
  H15      -0.4149138447    -2.8785957266    -2.7836278102
  C13       0.5856904186    -1.1603387810    -0.5057289256
  H17       1.6214401972    -2.9435364176    -0.9056763300
  C14       1.1494016877    -1.0542200362     0.8711955016
  C15       2.2399866250    -0.9544607911     3.4288475176
  C16       0.9442431964    -2.0981520429     1.7882413001
  C17       1.9061018996     0.0435783824     1.2473305571
  C18       2.4523571366     0.0895843476     2.5159373960
  C19       1.4845067753    -2.0486576226     3.0605260923
  H20       0.3500797578    -2.9443013764     1.4969449626
  H21       2.0514981867     0.8569289073     0.5508861050
  H22       3.0332039348     0.9425542182     2.8060617316
  H23       1.3130260427    -2.8586745195     3.7602037767
  H24       2.6630352826    -0.9064170758     4.4213930318

  nuclear repulsion energy.......  1590.011316833 hartrees
```

```
 ------------------------------------------------
/  end of geometry optimization iteration   5   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.722E-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        H1     C1     H2     C2     C3     C4     C5     C6
 grid # 1       73     87     73     87     89     89     84     84
 grid # 2      118     97    118     97    100     99     93     94
 grid # 3      223    182    216    182    195    197    182    180
 grid # 4      223    329    218    326    338    339    318    315

 number of gridpoints:
    atom        C7     O3     C8     H6     H7     C9     O2     O1
 grid # 1       85    111     86     73     73     80    111    107
 grid # 2       92    122     95    118    118     90    123    117
 grid # 3      185    250    185    216    224    166    268    245
 grid # 4      325    441    331    217    224    287    466    438

 number of gridpoints:
    atom       C11    C12    H14    H15    C13    H17    C14    C15
 grid # 1       77     86     70     69     92     71     88     88
 grid # 2       86     94    112    111    100    114     97     96
 grid # 3      155    182    218    222    194    218    195    183
 grid # 4      282    326    217    224    337    216    339    329

 number of gridpoints:
    atom       C16    C17    C18    C19    H20    H21    H22    H23
 grid # 1       86     88     88     89     71     72     73     73
 grid # 2       95     96     96     96    115    115    118    118
 grid # 3      183    181    185    182    217    220    222    224
 grid # 4      327    327    328    327    217    218    223    223

 number of gridpoints:
```

```
   atom       H24  total
 grid # 1      73   2746
 grid # 2     118   3468
 grid # 3     222   6699
 grid # 4     223   9818

 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  -913.10866875243           7.1E-04  2.9E-02
etot  2  Y  Y  6  M  -913.20400410821  9.5E-02  3.3E-04  1.2E-02
etot  3  N  Y  2  U  -913.21732861800  1.3E-02  9.2E-05  3.0E-03
etot  4  Y  Y  6  M  -913.21815872278  8.3E-04  3.8E-05  1.0E-03
etot  5  Y  Y  6  M  -913.21831326181  1.5E-04  1.4E-05  2.8E-04
etot  6  N  Y  2  U  -913.21832803305  1.5E-05  6.3E-06  7.4E-05
etot  7  Y  Y  6  M  -913.21832750010 -5.3E-07  1.9E-06  3.9E-05
etot  8  Y  N  6  M  -913.21832658730 -9.1E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1590.01131683301
   (E)  Total one-electron terms..... -4403.45456961476
   (I)  Total two-electron terms.....  1900.22492619446
   (L)  Electronic energy..... -2503.22964342031  (E+I)
   (N)  Total energy.............  -913.21832658730  (A+L)

 SCFE: SCF energy: HF    -913.21832658730 hartrees   iterations:   8


 HOMO energy:    -0.29245
 LUMO energy:     0.08120

  Orbital energies:
  -20.62595  -20.60051  -20.53939  -11.37645  -11.33054  -11.32138
  -11.29639  -11.27562  -11.26292  -11.25637  -11.25377  -11.25107
  -11.24392  -11.23758  -11.23703  -11.23674  -11.22520  -11.22477
  -11.22399  -11.22345  -11.22295   -1.49298   -1.43551   -1.39502
```

```
 -1.18177   -1.15609   -1.12257   -1.10309   -1.03947   -1.03346
 -1.01143   -1.00305   -0.93177   -0.89048   -0.87850   -0.87146
 -0.82228   -0.81500   -0.77267   -0.75082   -0.72526   -0.70844
 -0.68919   -0.68800   -0.67162   -0.66486   -0.65985   -0.63782
 -0.63050   -0.61946   -0.61702   -0.61126   -0.59063   -0.58200
 -0.57355   -0.56466   -0.54732   -0.54569   -0.52264   -0.52039
 -0.50357   -0.49156   -0.48648   -0.48177   -0.46328   -0.44193
 -0.43425   -0.39830   -0.33052   -0.32506   -0.30962   -0.29245
  0.08120    0.10803    0.14339    0.15206    0.16697    0.21840
  0.23349    0.24746    0.25421    0.26111

 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	H1	7.539897E-05	-2.994089E-04	1.831376E-03
2	C1	8.546777E-04	-1.732074E-03	-2.142410E-03
3	H2	1.898911E-03	-3.136550E-03	1.457312E-03
4	C2	-1.599404E-03	2.112524E-03	-2.119453E-03
5	C3	-1.794328E-03	1.283823E-03	-3.805736E-03
6	C4	2.658612E-04	-8.334449E-04	-2.265244E-03
7	C5	1.470538E-03	5.736181E-04	-6.408588E-03
8	C6	7.555509E-04	-8.873122E-04	-4.038311E-03
9	C7	-1.253150E-03	4.093952E-03	-9.115580E-03
10	O3	-3.317063E-03	8.344256E-03	5.759205E-03
11	C8	-5.935425E-03	6.974838E-04	4.203520E-03
12	H6	1.072995E-03	-1.738832E-03	-1.466022E-04
13	H7	2.233187E-03	-2.712811E-03	-4.235242E-04
14	C9	5.820199E-03	7.047273E-03	-4.089522E-02
15	O2	1.139131E-03	-6.474942E-03	6.028185E-02
16	O1	-6.963917E-03	2.446757E-03	-3.790414E-03
17	C11	1.086418E-03	-4.901901E-03	-5.160740E-03
18	C12	3.432240E-04	2.396767E-03	5.598118E-03
19	H14	1.962342E-04	-2.544889E-03	1.464610E-03
20	H15	-1.174060E-03	-8.931084E-04	5.084229E-04

```
 21    C13     6.814025E-03  -7.341249E-03  -2.601394E-03
 22    H17    -2.728523E-03   3.375566E-03  -1.690047E-03
 23    C14    -7.537451E-03  -1.332396E-02   8.519531E-03
 24    C15     5.993157E-03   1.167367E-02  -3.283906E-03
 25    C16     6.535342E-04   7.271515E-03  -1.142559E-02
 26    C17     1.092322E-03  -1.271755E-04   2.908157E-03
 27    C18    -1.546495E-03  -7.723104E-03   8.939587E-03
 28    C19     2.540148E-04  -2.069657E-03   1.297823E-03
 29    H20    -1.327364E-03  -8.799016E-05  -1.157335E-03
 30    H21     1.039350E-03  -2.339152E-03   3.125421E-03
 31    H22     2.150186E-03   1.793619E-03   1.841285E-03
 32    H23     5.703143E-04   4.477950E-03  -4.191262E-03
 33    H24    -5.291138E-04   1.749776E-03  -3.277951E-03
-----------   -------------  -------------  -------------
   total       7.293371E-05   1.709935E-04  -2.030888E-04

 end of program der1b


 start of program geopt   6

 geometry optimization step  6
 [ 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
 ** restarting optimization from step    5 **


 energy change:           2.9168E-03 .  (  5.0000E-05 )
 gradient maximum:        1.5155E-02 .  (  4.5000E-04 )
 gradient rms:            2.7232E-03 .  (  3.0000E-04 )
 step size:   0.12637  trust radius:   0.15000
 displacement maximum:    6.4675E-02 .  (  1.8000E-03 )
 displacement rms:        1.1536E-02 .  (  1.2000E-03 )
 predicted energy change:    -9.4284E-04    geom step:   1.2637E-01
full step:   1.2637E-01
 molecular structure not yet converged...

 center of mass moved by:
    x:     4.4409E-16     y:     1.1102E-16     z:     2.4286E-16

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -0.9635149338      0.9663825431     -4.2703493941
 C1       -0.9839694184      0.9666404511     -3.1970058083
```

```
 H2       -2.1991419660      2.6984393939     -2.9922409244
 C2       -1.6652188949      1.9176137164     -2.4798347946
 C3       -0.2498223652     -0.0889872241     -1.1183194062
 C4       -1.6989306378      1.8719868567     -1.0853546014
 C5       -0.3064244954     -0.0391204719     -2.5136292715
 C6       -0.9998968507      0.8665415766     -0.4280773511
 C7       -2.4340462691      2.8187248605     -0.2721136083
 O3        0.3276615339     -0.9550420153     -3.2591666293
 C8       -2.4514193700      2.7116189142      1.0530843871
 H6       -2.9670563655      3.6124729751     -0.7640098988
 H7       -2.9885216167      3.3812739131      1.6955656448
 C9       -1.7349274945      1.6253813501      1.7180804850
 O2       -1.7182289412      1.4382781277      2.8871081697
 O1       -1.0414503692      0.7826513764      0.9155069846
 C11       0.4801669362     -2.2473686503     -2.6968651049
 C12       0.9503889716     -2.1651280598     -1.2752978750
 H14       1.2108496590     -2.7475532139     -3.3179926325
 H15      -0.4655760659     -2.7888698929     -2.7830532480
 C13       0.6101528861     -1.1387244264     -0.5068126216
 H17       1.6029123555     -2.9367993014     -0.9072450813
 C14       1.1744535246     -1.0243721705      0.8735768486
 C15       2.3349909586     -0.8931510432      3.4049545981
 C16       0.8650204329     -1.9717475423      1.8431776589
 C17       2.0743540695     -0.0089644694      1.1830955807
 C18       2.6537846193      0.0532838730      2.4378978086
 C19       1.4392476060     -1.9037235316      3.1039618716
 H20       0.1639388972     -2.7553000910      1.6133707406
 H21       2.3275678339      0.7256157033      0.4376069078
 H22       3.3532999200      0.8393465916      2.6652736585
 H23       1.1801828071     -2.6365252712      3.8470580689
 H24       2.7830991621     -0.8386576586      4.3824484201

 nuclear repulsion energy.......  1585.879807682 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   6   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.772E-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        H1     C1     H2     C2     C3     C4     C5     C6
grid # 1       73     87     73     87     89     93     86     84
grid # 2      118     97    118     97    100    101     94     93
grid # 3      223    182    218    183    195    198    183    182
grid # 4      223    328    218    328    338    339    311    318

number of gridpoints:
   atom        C7     O3     C8     H6     H7     C9     O2     O1
grid # 1       85    111     88     73     73     79    111    108
grid # 2       93    120     95    118    118     89    123    117
grid # 3      186    248    185    218    224    168    270    245
grid # 4      326    442    331    218    224    283    465    438

number of gridpoints:
   atom       C11    C12    H14    H15    C13    H17    C14    C15
grid # 1       77     86     70     71     92     72     92     88
grid # 2       85     94    112    112    100    114    100     96
grid # 3      156    182    219    222    194    219    194    183
grid # 4      283    326    218    226    338    218    341    327

number of gridpoints:
   atom       C16    C17    C18    C19    H20    H21    H22    H23
grid # 1       87     88     88     88     72     73     73     73
grid # 2       95     96     96     96    115    117    118    118
grid # 3      183    182    184    183    218    220    221    222
grid # 4      328    327    327    327    218    220    223    223

number of gridpoints:
   atom       H24  total
grid # 1       73   2763
grid # 2      118   3473
grid # 3      223   6713
grid # 4      223   9823

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  -913.16498171474                5.0E-04  2.3E-02
etot  2  Y  Y  6  M  -913.21460160220  5.0E-02  2.4E-04  9.5E-03
etot  3  N  Y  2  U  -913.22167825923  7.1E-03  6.7E-05  2.4E-03
etot  4  Y  Y  6  M  -913.22212360364  4.5E-04  3.1E-05  8.7E-04
etot  5  Y  Y  6  M  -913.22221835063  9.5E-05  1.1E-05  1.9E-04
etot  6  N  Y  2  U  -913.22222149603  3.1E-06  4.6E-06  6.7E-05
etot  7  Y  N  6  M  -913.22222314111  1.6E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1585.87980768235
   (E)  Total one-electron terms..... -4395.18949675039
   (I)  Total two-electron terms.....  1896.08746592693
   (L)  Electronic energy............. -2499.10203082346  (E+I)
   (N)  Total energy.................  -913.22222314111  (A+L)

 SCFE: SCF energy: HF    -913.22222314111 hartrees   iterations:   7


 HOMO energy:    -0.29603
 LUMO energy:     0.07912

  Orbital energies:
  -20.62877  -20.60130  -20.53757  -11.38035  -11.33216  -11.32138
  -11.29992  -11.27740  -11.26379  -11.25724  -11.25482  -11.25277
  -11.24506  -11.23827  -11.23815  -11.23704  -11.22540  -11.22462
  -11.22410  -11.22352  -11.22255   -1.48780   -1.43602   -1.37831
   -1.18237   -1.15699   -1.12158   -1.10357   -1.03867   -1.03611
   -1.00941   -1.00710   -0.93269   -0.89282   -0.87878   -0.87113
   -0.82167   -0.81827   -0.77286   -0.75140   -0.72562   -0.70925
   -0.68977   -0.68830   -0.67085   -0.66230   -0.65907   -0.63642
   -0.62925   -0.62018   -0.61684   -0.61263   -0.59204   -0.57907
   -0.57648   -0.56433   -0.54833   -0.54418   -0.52146   -0.51851
   -0.50144   -0.49071   -0.48708   -0.48330   -0.46179   -0.44029
   -0.43143   -0.39756   -0.33060   -0.32605   -0.31245   -0.29603
    0.07912    0.10850    0.14474    0.15099    0.16349    0.21328
    0.23450    0.24691    0.25461    0.26189

 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	H1	-1.536869E-04	6.963907E-06	1.858001E-04
2	C1	-4.771373E-04	9.134958E-04	-1.885178E-05
3	H2	-1.393673E-04	1.432666E-04	-6.750562E-05
4	C2	-1.032321E-04	5.935401E-05	2.674348E-04
5	C3	4.598100E-04	-2.625245E-04	-4.912869E-04
6	C4	-2.382520E-04	7.781098E-04	-2.228338E-03
7	C5	2.933554E-04	-5.382457E-04	8.320209E-04
8	C6	1.041486E-03	-1.162280E-03	2.110019E-05
9	C7	1.134836E-04	1.428671E-04	-3.513037E-04
10	O3	8.862031E-04	-2.711543E-03	1.323005E-03
11	C8	-1.836894E-03	7.879979E-04	2.388004E-04
12	H6	-5.055134E-04	5.351101E-04	-5.573728E-04
13	H7	3.349327E-04	2.653667E-04	-1.737532E-04
14	C9	5.801019E-04	7.604366E-04	3.511279E-03
15	O2	1.619437E-04	-4.428214E-04	-1.348612E-03
16	O1	5.488343E-04	-1.590903E-03	-6.000165E-04
17	C11	-1.145436E-03	1.344777E-04	-1.129581E-03
18	C12	-3.516471E-04	7.802556E-04	4.154974E-04
19	H14	-6.918974E-04	9.327214E-05	2.441823E-05
20	H15	1.622028E-03	1.717443E-03	2.652508E-04
21	C13	-4.060071E-04	-9.388507E-04	-3.578458E-04
22	H17	-1.132050E-04	9.348690E-05	-1.204463E-04
23	C14	-2.064104E-04	-1.357006E-03	1.774010E-03
24	C15	1.124606E-03	1.617481E-03	-1.257692E-03
25	C16	3.512507E-04	1.194220E-03	-1.773464E-03
26	C17	-1.976957E-04	-3.543045E-04	7.210367E-04
27	C18	-4.223979E-04	-7.489982E-04	1.595079E-03
28	C19	-2.248315E-05	4.032974E-04	-9.170018E-04
29	H20	1.965618E-04	5.129542E-04	5.358794E-05
30	H21	-2.179642E-04	-1.395147E-04	1.841856E-04
31	H22	-2.553257E-04	-2.401552E-04	-1.421745E-04
32	H23	6.274145E-05	-2.850262E-04	3.174666E-04
33	H24	-3.960095E-04	9.038830E-05	-6.142747E-04
total		-1.032239E-04	2.580722E-04	-4.195484E-04

```
  end of program der1b


  start of program geopt   7

  geometry optimization step  7
  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:    0.2121473
   Cos(theta):   0.3131092

   Final level shift:  -5.3477210E-03

  energy change:          -9.7977E-04 .  (  5.0000E-05 )
  gradient maximum:        2.8822E-03 .  (  4.5000E-04 )
  gradient rms:            7.8689E-04 .  (  3.0000E-04 )
  step size:   0.21214  trust radius:   0.21213
  displacement maximum:    1.7374E-01 .  (  1.8000E-03 )
  displacement rms:        1.9366E-02 .  (  1.2000E-03 )
  predicted energy change:    -4.0663E-04    geom step:   2.1214E-01
full step:   2.1214E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -8.4153E-03     y:    -7.0404E-03     z:    -1.2512E-03

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -0.8710009816     0.9988122242    -4.2725039460
  C1       -0.9122220633     0.9954701124    -3.2001757714
  H2       -2.0708669361     2.7670784180    -3.0162466867
  C2       -1.5762638131     1.9651847530    -2.4949360733
  C3       -0.2524453793    -0.0915286035    -1.1107493827
  C4       -1.6454835773     1.9093443955    -1.1017975774
  C5       -0.2835681649    -0.0370915501    -2.5059757288
  C6       -0.9956093968     0.8753452975    -0.4337383791
  C7       -2.3743557955     2.8677742540    -0.2962614389
  O3        0.3306853331    -0.9798861624    -3.2325909216
  C8       -2.4396454847     2.7389027035     1.0279402486
  H6       -2.8645472011     3.6876133382    -0.7938302823
```

```
 H7       -2.9707718063      3.4182133371      1.6618297026
 C9       -1.7774637546      1.6196402823      1.7008155980
 O2       -1.8111439402      1.3980931148      2.8630374279
 O1       -1.0849441693      0.7713324814      0.9072539185
 C11       0.3974697726     -2.2830322665     -2.6609673092
 C12       0.8818894163     -2.2072895276     -1.2419343616
 H14       1.0917009959     -2.8466948902     -3.2825758654
 H15      -0.5907270646     -2.7585957626     -2.7302941365
 C13       0.5765234174     -1.1608589641     -0.4846494466
 H17       1.5121511100     -2.9929657948     -0.8687754966
 C14       1.1624235032     -1.0360375095      0.8861124068
 C15       2.3779335661     -0.8823196635      3.3927844838
 C16       1.0148941042     -2.0613932750      1.8119679327
 C17       1.9235983143      0.0704682710      1.2298605179
 C18       2.5312175769      0.1442747234      2.4718121591
 C19       1.6173997170     -1.9835264247      3.0602448017
 H20       0.4180624428     -2.9134762486      1.5584758686
 H21       2.0420896576      0.8685244733      0.5207907103
 H22       3.1213711829      1.0006920422      2.7217936234
 H23       1.4877062592     -2.7808829804      3.7698768779
 H24       2.8448246826     -0.8220209748      4.3596553583

 nuclear repulsion energy.......  1586.285383563 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   7   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.796E-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        H1     C1     H2     C2     C3     C4     C5     C6
 grid # 1       73     86     73     87     88     91     86     84
 grid # 2      118     97    118     97    100    101     94     94
 grid # 3      223    182    218    183    195    197    183    180
 grid # 4      223    327    218    328    339    342    309    314
```

number of gridpoints:

atom	C7	O3	C8	H6	H7	C9	O2	O1
grid # 1	86	110	88	73	73	79	111	107
grid # 2	93	120	95	118	118	89	123	117
grid # 3	186	249	185	218	224	168	270	245
grid # 4	326	442	332	218	224	284	464	440

number of gridpoints:

atom	C11	C12	H14	H15	C13	H17	C14	C15
grid # 1	78	86	70	71	91	72	92	89
grid # 2	90	94	112	112	100	114	100	96
grid # 3	159	182	219	222	194	218	195	182
grid # 4	285	326	223	228	339	216	340	327

number of gridpoints:

atom	C16	C17	C18	C19	H20	H21	H22	H23
grid # 1	87	88	88	89	71	72	73	73
grid # 2	95	96	96	96	115	115	118	118
grid # 3	183	183	184	182	216	219	221	222
grid # 4	327	326	327	327	217	217	223	223

number of gridpoints:

atom	H24	total
grid # 1	73	2758
grid # 2	118	3477
grid # 3	223	6710
grid # 4	223	9824

end of program grid

start of program rwr
end of program rwr

start of program scf

	iter	upd	dis	ic	gri d	total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	2	U	-913.17016902712		4.6E-04	2.2E-02
etot	2	Y	Y	6	M	-913.21483312519	4.5E-02	2.3E-04	9.1E-03
etot	3	N	Y	2	U	-913.22156334438	6.7E-03	7.6E-05	2.2E-03
etot	4	Y	Y	6	M	-913.22197752080	4.1E-04	1.7E-05	4.3E-04
etot	5	Y	Y	6	M	-913.22200565894	2.8E-05	9.8E-06	1.2E-04

```
etot   6  Y  Y  6  M  -913.22200622941  5.7E-07  3.2E-06  4.4E-05
etot   7  Y  N  6  M  -913.22200604137 -1.9E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1586.28538356292
   (E)  Total one-electron terms..... -4395.94009287358
   (I)  Total two-electron terms.....  1896.43270326928
   (L)  Electronic energy............. -2499.50738960429  (E+I)
   (N)  Total energy.................  -913.22200604137  (A+L)

 SCFE: SCF energy: HF    -913.22200604137 hartrees   iterations:   7


 HOMO energy:    -0.29525
 LUMO energy:     0.07851

  Orbital energies:
 -20.62892  -20.60154  -20.53751  -11.38056  -11.33255  -11.32201
 -11.30270  -11.27852  -11.26449  -11.25816  -11.25486  -11.25360
 -11.24587  -11.23907  -11.23813  -11.23716  -11.22483  -11.22455
 -11.22366  -11.22339  -11.22217   -1.48871   -1.43489   -1.37816
  -1.18275   -1.15842   -1.12163   -1.10361   -1.03818   -1.03694
  -1.01133   -1.00732   -0.93246   -0.89320   -0.87886   -0.87105
  -0.82379   -0.81849   -0.77287   -0.75203   -0.72593   -0.70969
  -0.69160   -0.68795   -0.67085   -0.66260   -0.65844   -0.63731
  -0.62909   -0.62147   -0.61706   -0.61213   -0.59339   -0.58009
  -0.57626   -0.56416   -0.54859   -0.54404   -0.52187   -0.51834
  -0.50167   -0.49329   -0.48741   -0.48374   -0.46250   -0.44065
  -0.43172   -0.39945   -0.33401   -0.32640   -0.31144   -0.29525
   0.07851    0.10670    0.14209    0.15010    0.16366    0.21695
   0.23406    0.24793    0.25329    0.26142

 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	H1	7.818437E-05	-2.179098E-04	-1.562386E-04
2	C1	9.545575E-04	-1.569608E-03	-5.016277E-04
3	H2	8.435671E-05	-3.874899E-04	5.422837E-04
4	C2	-3.966875E-04	8.814849E-04	1.293495E-03
5	C3	1.492583E-03	-1.698734E-03	-6.962417E-05
6	C4	-1.393651E-06	-9.547861E-05	-2.744323E-06
7	C5	7.453636E-04	-5.495401E-04	1.037599E-03
8	C6	-8.837972E-04	7.610165E-04	8.360094E-04
9	C7	-2.768211E-04	1.009003E-04	1.461628E-03
10	O3	8.305690E-04	-7.578640E-03	-3.927577E-04
11	C8	5.162559E-04	3.086831E-04	-1.288223E-03
12	H6	-7.341210E-05	-4.126550E-04	4.470072E-04
13	H7	-7.240170E-04	1.108276E-03	7.815027E-04
14	C9	-2.043633E-03	-7.931629E-05	1.961919E-03
15	O2	-3.337302E-04	2.016854E-03	-1.338201E-04
16	O1	2.069689E-03	-1.761133E-03	-4.086371E-03
17	C11	-1.200534E-03	2.782192E-04	-2.396867E-03
18	C12	-1.744972E-03	1.125390E-03	-8.555649E-04
19	H14	-4.233009E-03	4.085363E-03	2.474968E-03
20	H15	5.305147E-03	3.564517E-03	-3.239572E-04
21	C13	-3.634095E-04	-3.483331E-04	3.792658E-04
22	H17	8.345288E-04	-3.691350E-04	-3.465680E-04
23	C14	-3.068164E-03	-3.543218E-03	-5.914491E-04
24	C15	1.767317E-03	2.842993E-03	-3.912897E-04
25	C16	1.437706E-03	1.710129E-03	8.163996E-04
26	C17	2.600870E-03	1.577864E-03	3.558192E-03
27	C18	-2.001817E-03	-1.472396E-03	-2.022705E-03
28	C19	-2.455187E-03	-2.836303E-03	-2.872139E-03
29	H20	-2.291316E-03	-2.942075E-03	-3.586577E-04
30	H21	1.184743E-03	1.721314E-03	-2.159396E-04
31	H22	2.586540E-03	4.012094E-03	1.026364E-03
32	H23	-6.226186E-04	-7.560905E-04	-1.899139E-04
33	H24	3.427436E-04	8.475324E-04	6.312775E-05
total		1.166360E-04	3.245778E-04	-5.166973E-04

```
 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    7 **


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.1060785
   Cos(theta):   0.5871078

   Final level shift:  -2.1530890E-02

  energy change:           2.1710E-04 .  (  5.0000E-05 )
  gradient maximum:        2.8822E-03 .  (  4.5000E-04 )
  gradient rms:            7.8689E-04 .  (  3.0000E-04 )
  step size:   0.10608  trust radius:   0.10607
  displacement maximum:    6.7614E-02 .  (  1.8000E-03 )
  displacement rms:        9.6836E-03 .  (  1.2000E-03 )
  predicted energy change:    -3.8956E-04    geom step:   1.0608E-01
full step:   1.0608E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -7.7716E-16     y:     8.3267E-17     z:    -4.8572E-16

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -0.9386973544     0.9674513430    -4.2675114210
  C1       -0.9633969787     0.9686620333    -3.1951720111
  H2       -2.1243550691     2.7389738271    -3.0003518241
  C2       -1.6197245452     1.9414519069    -2.4842676270
  C3       -0.2696158051    -0.1087295435    -1.1136502964
  C4       -1.6661834452     1.8953080561    -1.0918834872
  C5       -0.3178940531    -0.0589401978    -2.5085666059
  C6       -1.0053878877     0.8621324552    -0.4295016371
  C7       -2.3823290375     2.8596486206    -0.2777680115
  O3        0.3012796246    -0.9892764903    -3.2476552731
  C8       -2.4296136894     2.7402010914     1.0487095396
  H6       -2.8833131179     3.6746673650    -0.7717383200
  H7       -2.9445005295     3.4287815885     1.6882019661
  C9       -1.7559268743     1.6220833297     1.7176427193
  O2       -1.7798894004     1.4009871659     2.8792492931
  O1       -1.0748198999     0.7646846144     0.9099561560
  C11       0.4513067467    -2.2712812017    -2.6865275999
  C12       0.9214265585    -2.1873250617    -1.2656721814
  H14       1.1722603935    -2.7750351613    -3.3076667206
  H15      -0.4864521628    -2.8044364743    -2.7679096720
  C13       0.5785651699    -1.1671912554    -0.4957669402
```

```
 H17       1.5706259888     -2.9591609260     -0.8983611574
 C14       1.1585344629     -1.0467639183      0.8792929794
 C15       2.3459048532     -0.8777600033      3.3940059589
 C16       0.9372846006     -2.0360279707      1.8238233536
 C17       1.9769357068      0.0329430610      1.2068788124
 C18       2.5694278737      0.1161436824      2.4548606176
 C19       1.5289068461     -1.9532285984      3.0766800635
 H20       0.2922956248     -2.8645414377      1.5858274982
 H21       2.1529801017      0.8094037445      0.4778165070
 H22       3.2045724859      0.9551334624      2.6888649169
 H23       1.3464649667     -2.7289115458      3.8064237590
 H24       2.7972540459     -0.8138305674      4.3661361435

 nuclear repulsion energy.......  1585.945922241 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   8   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    2.799E-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        H1     C1     H2     C2     C3     C4     C5     C6
 grid # 1       73     87     73     87     89     89     85     84
 grid # 2      118     97    118     97    100     99     94     94
 grid # 3      223    182    218    183    196    198    183    181
 grid # 4      223    328    218    328    339    338    313    315

 number of gridpoints:
    atom        C7     O3     C8     H6     H7     C9     O2     O1
 grid # 1       85    111     88     73     73     80    111    107
 grid # 2       93    120     95    118    118     89    123    117
 grid # 3      186    249    185    218    224    168    270    245
 grid # 4      326    441    332    218    224    284    465    439

 number of gridpoints:
```

atom	C11	C12	H14	H15	C13	H17	C14	C15
grid # 1	77	86	70	69	92	72	90	89
grid # 2	86	94	112	111	100	114	99	96
grid # 3	153	182	218	222	195	219	196	183
grid # 4	277	325	218	220	339	217	339	327

number of gridpoints:

atom	C16	C17	C18	C19	H20	H21	H22	H23
grid # 1	87	88	88	88	71	72	73	73
grid # 2	95	96	96	96	115	116	118	118
grid # 3	183	183	183	184	218	220	222	222
grid # 4	327	326	327	327	218	219	223	223

number of gridpoints:

atom	H24	total
grid # 1	73	2753
grid # 2	118	3470
grid # 3	222	6714
grid # 4	223	9806

end of program grid

start of program rwr
end of program rwr

start of program scf

	iter	updi	diis	icut	grid	total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	2	U	-913.21075987798		2.2E-04	1.1E-02
etot	2	Y	Y	6	M	-913.22057975480	9.8E-03	1.1E-04	4.2E-03
etot	3	N	Y	2	U	-913.22194559684	1.4E-03	3.1E-05	1.1E-03
etot	4	Y	Y	6	M	-913.22203290430	8.7E-05	1.4E-05	4.0E-04
etot	5	Y	Y	6	M	-913.22204967535	1.7E-05	4.6E-06	9.2E-05
etot	6	Y	N	6	M	-913.22205120951	1.5E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1585.94592224106	
(E)	Total one-electron terms.....	-4395.28517744085	
(I)	Total two-electron terms.....	1896.11720399029	
(L)	Electronic energy.....	-2499.16797345057	(E+I)
(N)	Total energy.....	-913.22205120951	(A+L)

```
SCFE: SCF energy: HF    -913.22205120951 hartrees   iterations:   6


HOMO energy:    -0.29523
LUMO energy:     0.07898

 Orbital energies:
 -20.62816  -20.60131  -20.53925  -11.38194  -11.33237  -11.32207
 -11.29716  -11.27870  -11.26374  -11.25697  -11.25452  -11.25304
 -11.24653  -11.23848  -11.23820  -11.23575  -11.22574  -11.22548
 -11.22457  -11.22392  -11.22271   -1.48644   -1.43908   -1.37990
  -1.18181   -1.15737   -1.12102   -1.10370   -1.03963   -1.03563
  -1.00927   -1.00751   -0.93394   -0.89232   -0.87867   -0.87042
  -0.82183   -0.81857   -0.77336   -0.75103   -0.72616   -0.70944
  -0.69072   -0.68922   -0.67147   -0.66311   -0.65900   -0.63662
  -0.62883   -0.62072   -0.61752   -0.61266   -0.59265   -0.57817
  -0.57777   -0.56438   -0.54854   -0.54444   -0.52130   -0.51842
  -0.50196   -0.49178   -0.48684   -0.48354   -0.46181   -0.44093
  -0.43213   -0.39820   -0.33130   -0.32704   -0.31134   -0.29523
   0.07898    0.10859    0.14306    0.15091    0.16334    0.21593
   0.23451    0.24657    0.25472    0.26211

 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    H1      1.293137E-04  -2.943201E-05  -5.748750E-04
  2    C1      2.714172E-04  -1.112221E-03   1.326574E-05
  3    H2     -1.294880E-04   1.207323E-04  -2.699133E-04
  4    C2      2.371580E-04  -1.719073E-04  -1.024347E-04
  5    C3      3.881080E-04  -3.476703E-04   4.552781E-04
  6    C4     -3.089156E-05  -1.075963E-03   2.725298E-03
  7    C5      4.109537E-04   1.208367E-03   7.360308E-04
  8    C6     -6.437137E-04   8.800598E-04  -1.630000E-03
```

9	C7	-2.253884E-04	-1.068627E-03	1.190118E-03
10	O3	7.117635E-05	5.050978E-03	-2.959201E-03
11	C8	2.928168E-03	-7.466288E-04	-1.238725E-03
12	H6	1.373412E-04	-5.883163E-05	9.536476E-05
13	H7	-6.195711E-04	1.411110E-04	9.449685E-05
14	C9	-2.417069E-03	-1.897881E-03	-2.704458E-03
15	O2	1.010246E-03	1.464230E-03	-3.910723E-04
16	O1	-2.832585E-04	1.411142E-03	2.719486E-03
17	C11	1.861307E-03	-1.158391E-05	3.489057E-03
18	C12	-1.926408E-04	-3.359170E-03	-1.636320E-03
19	H14	2.449910E-03	-1.700170E-03	-1.363068E-03
20	H15	-5.371327E-03	-2.623135E-03	-9.017966E-05
21	C13	3.948353E-04	4.209816E-03	1.610446E-03
22	H17	1.283369E-03	-8.511582E-04	3.354198E-04
23	C14	-1.047893E-03	4.123142E-03	-1.774649E-03
24	C15	-2.595660E-03	-3.998798E-03	2.527070E-06
25	C16	7.878395E-04	-1.400652E-03	2.413456E-03
26	C17	-3.011100E-05	8.679593E-04	-1.499428E-03
27	C18	-1.888405E-04	1.299379E-03	-3.064855E-03
28	C19	1.005564E-03	-3.179000E-04	2.129561E-03
29	H20	5.564013E-04	6.225088E-04	2.238412E-04
30	H21	-3.781190E-04	-1.863940E-03	1.384425E-03
31	H22	-1.019896E-03	-1.298657E-03	1.253903E-04
32	H23	4.821482E-04	2.665077E-03	-2.088861E-03
33	H24	7.850165E-04	2.655806E-05	1.390223E-03
---		---	---	---
total		1.640586E-05	1.567350E-04	-2.543556E-04

 end of program der1b

 start of program geopt   9

 geometry optimization step 9
** stopping now - optimization seems to be stuck **

 ****
 **   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
 H1   -0.9386973544   0.9674513430   -4.2675114210

```
 C1       -0.9633969787      0.9686620333     -3.1951720111
 H2       -2.1243550691      2.7389738271     -3.0003518241
 C2       -1.6197245452      1.9414519069     -2.4842676270
 C3       -0.2696158051     -0.1087295435     -1.1136502964
 C4       -1.6661834452      1.8953080561     -1.0918834872
 C5       -0.3178940531     -0.0589401978     -2.5085666059
 C6       -1.0053878877      0.8621324552     -0.4295016371
 C7       -2.3823290375      2.8596486206     -0.2777680115
 O3        0.3012796246     -0.9892764903     -3.2476552731
 C8       -2.4296136894      2.7402010914      1.0487095396
 H6       -2.8833131179      3.6746673650     -0.7717383200
 H7       -2.9445005295      3.4287815885      1.6882019661
 C9       -1.7559268743      1.6220833297      1.7176427193
 O2       -1.7798894004      1.4009871659      2.8792492931
 O1       -1.0748198999      0.7646846144      0.9099561560
 C11       0.4513067467     -2.2712812017     -2.6865275999
 C12       0.9214265585     -2.1873250617     -1.2656721814
 H14       1.1722603935     -2.7750351613     -3.3076667206
 H15      -0.4864521628     -2.8044364743     -2.7679096720
 C13       0.5785651699     -1.1671912554     -0.4957669402
 H17       1.5706259888     -2.9591609260     -0.8983611574
 C14       1.1585344629     -1.0467639183      0.8792929794
 C15       2.3459048532     -0.8777600033      3.3940059589
 C16       0.9372846006     -2.0360279707      1.8238233536
 C17       1.9769357068      0.0329430610      1.2068788124
 C18       2.5694278737      0.1161436824      2.4548606176
 C19       1.5289068461     -1.9532285984      3.0766800635
 H20       0.2922956248     -2.8645414377      1.5858274982
 H21       2.1529801017      0.8094037445      0.4778165070
 H22       3.2045724859      0.9551334624      2.6888649169
 H23       1.3464649667     -2.7289115458      3.8064237590
 H24       2.7972540459     -0.8138305674      4.3661361435

 nuclear repulsion energy.......  1585.945922241 hartrees
 -----------------------------------------------
/  end of geometry optimization iteration   9   /
-----------------------------------------------

 end of program geopt


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

Total cpu seconds     user:    1006.172   user+sys:    1006.172
```