Process 0 of 1 is on clab-01 - thread support 0
initial socket setup ...start
initial socket setup ...done
now start server 0 ...
Q-Chem Developer Version!
Welcome to Q-Chem
A Quantum Leap Into The Future Of Chemistry

Q-Chem 5.1, Q-Chem, Inc., Pleasanton, CA (2018)

Yihan Shao, Zhengting Gan, E. Epifanovsky, A. T. B. Gilbert, M. Wormit,
J. Kussmann, A. W. Lange, A. Behn, Jia Deng, Xintian Feng, D. Ghosh,
M. Goldey, P. R. Horn, L. D. Jacobson, I. Kaliman, T. Kus, A. Landau,
Jie Liu, E. I. Proynov, R. M. Richard, R. P. Steele, E. J. Sundstrom,
H. L. Woodcock III, P. M. Zimmerman, D. Zuev, B. Albrecht, E. Alguire,
S. A. Baeppler, D. Barton, Z. Benda, Y. A. Bernard, E. J. Berquist,
K. B. Bravaya, H. Burton, D. Casanova, Chun-Min Chang, Yunqing Chen,
A. Chien, K. D. Closser, M. P. Coons, S. Coriani, S. Dasgupta,
A. L. Dempwolff, M. Diedenhofen, Hainam Do, R. G. Edgar, Po-Tung Fang,
S. Faraji, S. Fatehi, Qingguo Feng, K. D. Fenk, J. Fosso-Tande,
Qinghui Ge, A. Ghysels, G. Gidofalvi, J. Gomes, J. Gonthier, A. Gunina,
D. Hait, M. W. D. Hanson-Heine, P. H. P. Harbach, A. W. Hauser,
J. E. Herr, E. G. Hohenstein, Z. C. Holden, Kerwin Hui, B. C. Huynh,
T.-C. Jagau, Hyunjun Ji, B. Kaduk, K. Khistyaev, Jaehoon Kim,
P. Klunzinger, K. Koh, D. Kosenkov, L. Koulias, T. Kowalczyk,
C. M. Krauter, A. Kunitsa, Ka Un Lao, A. Laurent, K. V. Lawler,
Joonho Lee, D. Lefrancois, S. Lehtola, D. S. Levine, Yi-Pei Li,
You-Sheng Lin, Fenglai Liu, E. Livshits, A. Luenser, P. Manohar,
E. Mansoor, S. F. Manzer, Shan-Ping Mao, Yuezhi Mao, N. Mardirossian,
A. V. Marenich, T. Markovich, L. A. Martinez-Martinez, S. A. Maurer,
N. J. Mayhall, S. C. McKenzie, J.-M. Mewes, A. F. Morrison,
J. W. Mullinax, K. Nanda, T. S. Nguyen-Beck, R. Olivares-Amaya,
J. A. Parkhill, T. M. Perrine, F. Plasser, P. Pokhilko, S. Prager,
A. Prociuk, E. Ramos, D. R. Rehn, F. Rob, M. Schneider, N. Sergueev,

S. M. Sharada, S. Sharma, D. W. Small, T. Stauch, T. Stein,
Yu-Chuan Su, A. J. W. Thom, A. Tkatchenko, T. Tsuchimochi, N. M. Tubman,
L. Vogt, M. L. Vidal, O. Vydrov, M. A. Watson, J. Wenzel,
M. de Wergifosse, T. A. Wesolowski, A. White, J. Witte, A. Yamada,
Jun Yang, K. Yao, S. Yeganeh, S. R. Yost, Zhi-Qiang You, A. Zech,
Igor Ying Zhang, Xing Zhang, Yan Zhao, Ying Zhu, B. R. Brooks,
G. K. L. Chan, C. J. Cramer, M. S. Gordon, W. J. Hehre, A. Klamt,
M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Aspuru-Guzik, R. Baer,
A. T. Bell, N. A. Besley, Jeng-Da Chai, A. E. DePrince, III,
R. A. DiStasio Jr., A. Dreuw, B. D. Dunietz, T. R. Furlani,
Chao-Ping Hsu, Yousung Jung, Jing Kong, D. S. Lambrecht, WanZhen Liang,
C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik,
T. Van Voorhis, J. M. Herbert, A. I. Krylov, P. M. W. Gill, M. Head-Gordon

Contributors to earlier versions of Q-Chem not listed above:
R. D. Adamson, B. Austin, J. Baker, G. J. O. Beran, K. Brandhorst,
S. T. Brown, E. F. C. Byrd, A. K. Chakraborty, C.-L. Cheng,
Siu Hung Chien, D. M. Chipman, D. L. Crittenden, H. Dachsel,
R. J. Doerksen, A. D. Dutoi, L. Fusti-Molnar, W. A. Goddard III,
A. Golubeva-Zadorozhnaya, S. R. Gwaltney, G. Hawkins, A. Heyden,
S. Hirata, G. Kedziora, F. J. Keil, C. Kelley, Jihan Kim, R. A. King,
R. Z. Khaliullin, P. P. Korambath, W. Kurlancheek, A. M. Lee, M. S. Lee,
S. V. Levchenko, Ching Yeh Lin, D. Liotard, R. C. Lochan, I. Lotan,
P. E. Maslen, N. Nair, D. P. O'Neill, D. Neuhauser, E. Neuscamman,
C. M. Oana, R. Olson, B. Peters, R. Peverati, P. A. Pieniazek,
Y. M. Rhee, J. Ritchie, M. A. Rohrdanz, E. Rosta, N. J. Russ,
H. F. Schaefer III, N. E. Schultz, N. Shenvi, A. C. Simmonett, A. Sodt,
D. Stuck, K. S. Thanthiriwatte, V. Vanovschi, Tao Wang, A. Warshel,
C. F. Williams, Q. Wu, X. Xu, W. Zhang

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Q-Chem 5.1.1 for Intel X86 EM64T Linux

```
 Parts of Q-Chem use Armadillo 8.300.2 (Tropical Shenanigans).
 http://arma.sourceforge.net/

 Q-Chem begins on Mon Jun  3 12:25:59 2019

Host:
0

     Scratch files written to /home/christian/scratch/qchem24662//
 Parallel job on  1  processors
Input Ideriv = 2
Curr. Ideriv = -1
Max.  Ideriv = 2

Checking the input file for inconsistencies...   ...done.

------------------------------------------------------------
User input:
------------------------------------------------------------
$molecule
0 1
  H    2.1445109   -0.0631326    0.0023074
  C    1.2918836    0.6181044   -0.0000933
  H    1.3442939    1.2712784    0.8804951
  H    1.3465972    1.2668926   -0.8838496
  C   -0.0000218   -0.1739255    0.0009136
  O    0.0000719   -1.4153943   -0.0002510
  C   -1.2919819    0.6180477   -0.0001134
  H   -1.3443717    1.2712177    0.8804504
  H   -1.3462794    1.2667052   -0.8839367
  H   -2.1446053   -0.0631662    0.0022997
$end

$rem
   BASIS  =  6-31G
   GUI  =  2
   JOB_TYPE  =  Optimization
   METHOD  =  B3LYP
   SCF_CONVERGENCE  =  8
   SYMMETRY_IGNORE  =  1
$end


------------------------------------------------------------
 ------------------------------------------------------------
            Standard Nuclear Orientation (Angstroms)
    I     Atom           X                Y                Z
 ------------------------------------------------------------
    1      H       2.1445109000    -0.0631326000     0.0023074000
```

```
    2      C       1.2918836000     0.6181044000    -0.0000933000
    3      H       1.3442939000     1.2712784000     0.8804951000
    4      H       1.3465972000     1.2668926000    -0.8838496000
    5      C      -0.0000218000    -0.1739255000     0.0009136000
    6      O       0.0000719000    -1.4153943000    -0.0002510000
    7      C      -1.2919819000     0.6180477000    -0.0001134000
    8      H      -1.3443717000     1.2712177000     0.8804504000
    9      H      -1.3462794000     1.2667052000    -0.8839367000
   10      H      -2.1446053000    -0.0631662000     0.0022997000
 ---------------------------------------------------------------
 Nuclear Repulsion Energy =   118.4763927948 hartrees
 There are       16 alpha and       16 beta electrons
 Requested basis set is 6-31G
 There are 24 shells and 48 basis functions

 Total QAlloc Memory Limit   2000 MB
 Mega-Array Size       188 MB
 MEM_STATIC part       192 MB
 A cutoff of  1.0D-11 yielded    297 shell pairs
 There are      1221 function pairs
 Smallest overlap matrix eigenvalue = 7.66E-03

 Scale SEOQF with 1.000000e-01/1.000000e+00/1.000000e+00

 Standard Electronic Orientation quadrupole field applied
 Nucleus-field energy     =     0.0000000174 hartrees
 Guess from superposition of atomic densities
 Warning:  Energy on first SCF cycle will be non-variational
 SAD guess density has 32.000000 electrons

 ------------------------------------------------------------------------
--
  General SCF calculation program by
  Eric Jon Sundstrom, Paul Horn, Yuezhi Mao, Dmitri Zuev, Alec White,
  David Stuck, Shaama M.S., Shane Yost, Joonho Lee, David Small,
  Daniel Levine, Susi Lehtola, Hugh Burton, Evgeny Epifanovsky
 ------------------------------------------------------------------------
--
 Exchange:     0.2000 Hartree-Fock + 0.0800 Slater + 0.7200 B88
 Correlation:  0.1900 VWN1RPA + 0.8100 LYP
 Using SG-1 standard quadrature grid
 A restricted SCF calculation will be
 performed using DIIS
 SCF converges when DIIS error is below 1.0e-08
 ---------------------------------------
  Cycle       Energy         DIIS error
 ---------------------------------------
    1    -193.6140088708      1.31e-01
    2    -192.9649945764      2.22e-02
```

```
   3    -192.7103619635      3.99e-02
   4    -193.0799361978      8.49e-03
   5    -193.0995647620      9.45e-04
   6    -193.0997570096      2.72e-04
   7    -193.0997778562      6.30e-05
   8    -193.0997788487      7.60e-06
   9    -193.0997788616      1.07e-06
  10    -193.0997788619      7.18e-08
  11    -193.0997788619      6.42e-09  Convergence criterion met
 ----------------------------------------
 SCF time:   CPU 2.91s  wall 3.00s
 SCF   energy in the final basis set =     -193.0997788619
 Total energy in the final basis set =     -193.0997788619

 -----------------------------------------------------------------

                   Orbital Energies (a.u.)
 -----------------------------------------------------------------

 Alpha MOs
 -- Occupied --
-19.139 -10.284 -10.189 -10.189  -1.047  -0.775  -0.717  -0.535
 -0.464  -0.463  -0.449  -0.408  -0.390  -0.382  -0.345  -0.247
 -- Virtual --
 -0.023   0.085   0.136   0.145   0.157   0.169   0.177   0.195
  0.285   0.319   0.507   0.540   0.581   0.591   0.596   0.686
  0.709   0.716   0.793   0.808   0.869   0.937   0.950   0.951
  0.954   0.978   0.995   1.031   1.150   1.246   1.446   1.785
 -----------------------------------------------------------------

          Ground-State Mulliken Net Atomic Charges

    Atom                 Charge (a.u.)
  ----------------------------------------
     1 H                     0.174381
     2 C                    -0.472529
     3 H                     0.159613
     4 H                     0.159890
     5 C                     0.362018
     6 O                    -0.404766
     7 C                    -0.472488
     8 H                     0.159617
     9 H                     0.159890
    10 H                     0.174376
  ----------------------------------------
  Sum of atomic charges =     0.000000

 -----------------------------------------------------------------
                   Cartesian Multipole Moments
```

```
 ---------------------------------------------------------------------
    Charge (ESU x 10^10)
                  0.0000
    Dipole Moment (Debye)
         X      -0.0001      Y       3.1673      Z      -0.0010
       Tot       3.1673
    Quadrupole Moments (Debye-Ang)
        XX     -23.4272     XY       0.0007     YY     -28.9971
        XZ      -0.0004     YZ      -0.0041     ZZ     -24.0785
    Octopole Moments (Debye-Ang^2)
       XXX       0.0005    XXY      -1.9003    XYY       0.0005
       YYY       3.6070    XXZ      -0.0066    XYZ      -0.0005
       YYZ       0.0029    XZZ      -0.0001    YZZ      -0.3274
       ZZZ      -0.0147
    Hexadecapole Moments (Debye-Ang^3)
      XXXX    -194.3247   XXXY       0.0026   XXYY     -57.1561
      XYYY       0.0014   YYYY    -152.8727   XXXZ      -0.0026
      XXYZ      -0.0201   XYYZ      -0.0007   YYYZ       0.0117
      XXZZ     -39.4007   XYZZ       0.0000   YYZZ     -26.9619
      XZZZ      -0.0003   YZZZ      -0.0134   ZZZZ     -35.5816
 ---------------------------------------------------------------------
 Calculating analytic gradient of the SCF energy
 Gradient of SCF Energy
           1           2           3           4           5
6
    1  -0.0000705   0.0001112  -0.0001162   0.0000135  -0.0000006
0.0000070
    2  -0.0000169  -0.0000603   0.0000145   0.0000552  -0.0000097
0.0000308
    3  -0.0000188  -0.0001289   0.0000577  -0.0000626
0.0004095  -0.0001193
           7           8           9          10
    1  -0.0001688   0.0001199   0.0000259   0.0000786
    2  -0.0000288  -0.0000007   0.0000311  -0.0000152
    3  -0.0001367   0.0000540  -0.0000494  -0.0000055
 Max gradient component =       4.095E-04
 RMS gradient           =       1.035E-04
 Gradient time:  CPU 0.43 s  wall 0.43 s
 Geometry Optimization Parameters
   NAtoms,    NIC,     NZ,  NCons,   NDum,   NFix, NCnnct, MaxDiis
       10      56       0       0       0       0       0       0


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES **
   Searching for a Minimum

   Optimization Cycle:   1

                      Coordinates (Angstroms)
```

ATOM		X	Y	Z
1	H	2.1445109000	-0.0631326000	0.0023074000
2	C	1.2918836000	0.6181044000	-0.0000933000
3	H	1.3442939000	1.2712784000	0.8804951000
4	H	1.3465972000	1.2668926000	-0.8838496000
5	C	-0.0000218000	-0.1739255000	0.0009136000
6	O	0.0000719000	-1.4153943000	-0.0002510000
7	C	-1.2919819000	0.6180477000	-0.0001134000
8	H	-1.3443717000	1.2712177000	0.8804504000
9	H	-1.3462794000	1.2667052000	-0.8839367000
10	H	-2.1446053000	-0.0631662000	0.0022997000

Point Group: c1 Number of degrees of freedom: 24

Energy is -193.099778862

Attempting to Generate Delocalized Internal Coordinates

24 Hessian modes will be used to form the next step
Hessian Eigenvalues:
0.007144 0.007145 0.007146 0.073153 0.073157
0.073565
0.073588 0.160000 0.160000 0.160000 0.160000
0.160000
0.160000 0.249999 0.250000 0.308157 0.308174
0.339378
0.339427 0.339442 0.339468 0.346561 0.346581
0.864700

Minimum Search - Taking Simple RFO Step
Searching for Lamda that Minimizes Along All modes
Value Taken Lamda = -0.00000296
Step Taken. Stepsize is 0.017787

	Maximum	Tolerance	Cnvgd?
Gradient	0.000155	0.000300	YES
Displacement	0.015090	0.001200	NO
Energy change	*********	0.000001	NO

New Cartesian Coordinates Obtained by Inverse Iteration

Displacement from previous Coordinates is: 0.010577

Standard Nuclear Orientation (Angstroms)

I	Atom	X	Y	Z
1	H	2.1448820902	-0.0631020475	0.0035452678

```
   2      C       1.2921109998     0.6180576928    -0.0002624385
   3      H       1.3435963065     1.2709554073     0.8804894377
   4      H       1.3487543381     1.2670729733    -0.8835682670
   5      C       0.0000132612    -0.1738409258    -0.0028883048
   6      O       0.0000535241    -1.4153229086     0.0010261887
   7      C      -1.2921201650     0.6180251666    -0.0003283144
   8      H      -1.3436356199     1.2709497842     0.8803966602
   9      H      -1.3486889018     1.2669852528    -0.8836768592
  10      H      -2.1448684333    -0.0631529950     0.0034888295
 ---------------------------------------------------------------
 Nuclear Repulsion Energy =   118.4701013278 hartrees
 There are       16 alpha and       16 beta electrons
 Applying Cartesian multipole field
    Component          Value
    ---------          -----
     (2,0,0)        1.00000E-11
     (0,2,0)        2.00000E-10
     (0,0,2)       -3.00000E-10
 Nucleus-field energy     =     0.0000000174 hartrees
 Requested basis set is 6-31G
 There are 24 shells and 48 basis functions
 A cutoff of  1.0D-11 yielded    297 shell pairs
 There are      1221 function pairs
 Smallest overlap matrix eigenvalue = 7.67E-03
 Guess MOs from SCF MO coefficient file

 ---------------------------------------------------------------------
--
  General SCF calculation program by
  Eric Jon Sundstrom, Paul Horn, Yuezhi Mao, Dmitri Zuev, Alec White,
  David Stuck, Shaama M.S., Shane Yost, Joonho Lee, David Small,
  Daniel Levine, Susi Lehtola, Hugh Burton, Evgeny Epifanovsky
 ---------------------------------------------------------------------
--
 Exchange:     0.2000 Hartree-Fock + 0.0800 Slater + 0.7200 B88
 Correlation:  0.1900 VWN1RPA + 0.8100 LYP
 Using SG-1 standard quadrature grid
 A restricted SCF calculation will be
 performed using DIIS
 SCF converges when DIIS error is below 1.0e-08
 ---------------------------------------
  Cycle       Energy         DIIS error
 ---------------------------------------
    1    -193.0997620572      1.48e-04
    2    -193.0997763617      1.75e-05
    3    -193.0997765265      2.58e-06
    4    -193.0997765284      1.80e-06
    5    -193.0997765292      8.05e-07
    6    -193.0997765293      4.27e-07
```

```
   7    -193.0997765294      3.43e-08
   8    -193.0997765294      1.37e-08
   9    -193.0997765294      1.73e-09  Convergence criterion met
 --------------------------------------
 SCF time:   CPU 2.41s  wall 2.00s
 SCF   energy in the final basis set =     -193.0997765294
 Total energy in the final basis set =     -193.0997765294

 -----------------------------------------------------------------

                   Orbital Energies (a.u.)
 -----------------------------------------------------------------

 Alpha MOs
 -- Occupied --
-19.139 -10.284 -10.189 -10.189  -1.047  -0.775  -0.717  -0.535
 -0.464  -0.463  -0.449  -0.408  -0.390  -0.382  -0.345  -0.247
 -- Virtual --
 -0.023   0.085   0.136   0.145   0.157   0.169   0.177   0.195
  0.285   0.319   0.507   0.540   0.581   0.591   0.597   0.686
  0.709   0.716   0.793   0.808   0.869   0.937   0.950   0.951
  0.954   0.978   0.995   1.032   1.150   1.246   1.445   1.785
 -----------------------------------------------------------------

          Ground-State Mulliken Net Atomic Charges

    Atom                  Charge (a.u.)
  ----------------------------------------
     1 H                     0.174377
     2 C                    -0.472625
     3 H                     0.159821
     4 H                     0.159729
     5 C                     0.362160
     6 O                    -0.404773
     7 C                    -0.472616
     8 H                     0.159820
     9 H                     0.159731
    10 H                     0.174376
  ----------------------------------------
  Sum of atomic charges =    -0.000000

 -----------------------------------------------------------------
                   Cartesian Multipole Moments
 -----------------------------------------------------------------
   Charge (ESU x 10^10)
                0.0000
   Dipole Moment (Debye)
        X      -0.0001      Y       3.1676      Z      -0.0043
      Tot       3.1676
```

```
    Quadrupole Moments (Debye-Ang)
        XX     -23.4221     XY       0.0003     YY     -28.9960
        XZ      -0.0000     YZ       0.0062     ZZ     -24.0795
    Octopole Moments (Debye-Ang^2)
       XXX      -0.0009    XXY      -1.8909    XYY      -0.0005
       YYY       3.6059    XXZ       0.0185    XYZ      -0.0000
       YYZ       0.0152    XZZ      -0.0004    YZZ      -0.3288
       ZZZ       0.0254
    Hexadecapole Moments (Debye-Ang^3)
      XXXX    -194.3762   XXXY       0.0007   XXYY     -57.1561
      XYYY       0.0007   YYYY    -152.8537   XXXZ      -0.0024
      XXYZ      -0.0065   XYYZ      -0.0008   YYYZ       0.0558
      XXZZ     -39.4099   XYZZ      -0.0000   YYZZ     -26.9603
      XZZZ      -0.0019   YZZZ       0.0179   ZZZZ     -35.5786
 -----------------------------------------------------------------
 Calculating analytic gradient of the SCF energy
 Gradient of SCF Energy
           1           2           3           4           5
6
    1  -0.0000052   0.0000498   0.0000441  -0.0000536   0.0000010
0.0000036
    2   0.0000064   0.0000081
0.0000450  -0.0000454  -0.0000322  -0.0000001
    3   0.0000119   0.0003554  -0.0000057   0.0000065  -0.0010700
0.0003319
           7           8           9          10
    1  -0.0000647  -0.0000434   0.0000597   0.0000088
    2   0.0000155   0.0000421  -0.0000472   0.0000077
    3   0.0003556  -0.0000060   0.0000058   0.0000146
 Max gradient component =       1.070E-03
 RMS gradient           =       2.262E-04
 Gradient time:  CPU 0.46 s  wall 0.45 s
 Geometry Optimization Parameters
   NAtoms,    NIC,     NZ,  NCons,   NDum,   NFix, NCnnct, MaxDiis
       10      56       0       0       0       0       0       0

 Cartesian Hessian Update
 Hessian Updated using BFGS Update


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES **
   Searching for a Minimum

   Optimization Cycle:   2

                     Coordinates (Angstroms)
     ATOM                X              Y              Z
      1  H         2.1448820902   -0.0631020475    0.0035452678
      2  C         1.2921109998    0.6180576928   -0.0002624385
```

```
     3  H         1.3435963065    1.2709554073    0.8804894377
     4  H         1.3487543381    1.2670729733   -0.8835682670
     5  C         0.0000132612   -0.1738409258   -0.0028883048
     6  O         0.0000535241   -1.4153229086    0.0010261887
     7  C        -1.2921201650    0.6180251666   -0.0003283144
     8  H        -1.3436356199    1.2709497842    0.8803966602
     9  H        -1.3486889018    1.2669852528   -0.8836768592
    10  H        -2.1448684333   -0.0631529950    0.0034888295
  Point Group: c1    Number of degrees of freedom:    24


  Energy is   -193.099776529

 Hessian Updated using BFGS Update

 20 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.006986    0.007145    0.028218    0.072863    0.073158
0.073573
     0.074115    0.144229    0.166574    0.248542    0.250004
0.307861
     0.308182    0.336454    0.339408    0.339457    0.339933
0.345798
     0.346570    0.864485

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda =  -0.00000593
 Step Taken.  Stepsize is  0.013937

                           Maximum     Tolerance    Cnvgd?
        Gradient          0.000399      0.000300      NO
        Displacement      0.011493      0.001200      NO
        Energy change     0.000002      0.000001      NO


 New Cartesian Coordinates Obtained by Inverse Iteration

 Displacement from previous Coordinates is:  0.010719
 ---------------------------------------------------------------------
            Standard Nuclear Orientation (Angstroms)
   I     Atom          X                Y                Z
 ---------------------------------------------------------------------
   1      H       2.1449253542    -0.0631099035     0.0018681857
   2      C       1.2921345557     0.6180544913    -0.0000941459
   3      H       1.3456873768     1.2709933373     0.8804766405
   4      H       1.3468864705     1.2670105261    -0.8835578787
   5      C       0.0000195544    -0.1738127406     0.0004077407
   6      O       0.0000459372    -1.4153034080     0.0007815543
```

```
   7      C      -1.2921253132     0.6180245485    -0.0001679677
   8      H      -1.3457185301     1.2709964802     0.8803751408
   9      H      -1.3468665092     1.2669397045    -0.8836678165
  10      H      -2.1448914963    -0.0631656358     0.0018007469
 ---------------------------------------------------------------
 Nuclear Repulsion Energy =   118.4697303982 hartrees
 There are       16 alpha and       16 beta electrons
 Applying Cartesian multipole field
    Component          Value
    ---------          -----
     (2,0,0)        1.00000E-11
     (0,2,0)        2.00000E-10
     (0,0,2)       -3.00000E-10
 Nucleus-field energy     =     0.0000000174 hartrees
 Requested basis set is 6-31G
 There are 24 shells and 48 basis functions
 A cutoff of  1.0D-11 yielded    297 shell pairs
 There are      1221 function pairs
 Smallest overlap matrix eigenvalue = 7.67E-03
 Guess MOs from SCF MO coefficient file

 ---------------------------------------------------------------------
--
  General SCF calculation program by
  Eric Jon Sundstrom, Paul Horn, Yuezhi Mao, Dmitri Zuev, Alec White,
  David Stuck, Shaama M.S., Shane Yost, Joonho Lee, David Small,
  Daniel Levine, Susi Lehtola, Hugh Burton, Evgeny Epifanovsky
 ---------------------------------------------------------------------
--
 Exchange:     0.2000 Hartree-Fock + 0.0800 Slater + 0.7200 B88
 Correlation:  0.1900 VWN1RPA + 0.8100 LYP
 Using SG-1 standard quadrature grid
 A restricted SCF calculation will be
 performed using DIIS
 SCF converges when DIIS error is below 1.0e-08
 ---------------------------------------
  Cycle       Energy         DIIS error
 ---------------------------------------
    1    -193.0997710240      1.13e-04
    2    -193.0997793807      1.28e-05
    3    -193.0997794728      2.09e-06
    4    -193.0997794726      2.86e-06
    5    -193.0997794744      4.42e-07
    6    -193.0997794745      6.40e-08
    7    -193.0997794745      2.39e-08
    8    -193.0997794745      5.60e-09  Convergence criterion met
 ---------------------------------------
 SCF time:   CPU 2.22s  wall 3.00s
 SCF   energy in the final basis set =     -193.0997794745
```

Total energy in the final basis set = -193.0997794745

Orbital Energies (a.u.)

Alpha MOs

-- Occupied --

-19.139	-10.284	-10.189	-10.189	-1.047	-0.775	-0.717	-0.535
-0.464	-0.463	-0.449	-0.408	-0.390	-0.382	-0.345	-0.247

-- Virtual --

-0.023	0.085	0.136	0.145	0.157	0.169	0.177	0.195
0.285	0.319	0.507	0.540	0.581	0.591	0.597	0.686
0.709	0.716	0.793	0.808	0.869	0.937	0.950	0.951
0.954	0.978	0.995	1.032	1.150	1.246	1.445	1.785

Ground-State Mulliken Net Atomic Charges

Atom	Charge (a.u.)
1 H	0.174376
2 C	-0.472638
3 H	0.159727
4 H	0.159833
5 C	0.362179
6 O	-0.404775
7 C	-0.472636
8 H	0.159725
9 H	0.159834
10 H	0.174376

Sum of atomic charges = -0.000000

Cartesian Multipole Moments

Charge (ESU x 10^10)

0.0000

Dipole Moment (Debye)

X	-0.0001	Y	3.1676	Z	-0.0025
Tot	3.1676				

Quadrupole Moments (Debye-Ang)

XX	-23.4213	XY	0.0002	YY	-28.9958
XZ	0.0000	YZ	0.0017	ZZ	-24.0796

Octopole Moments (Debye-Ang^2)

XXX	-0.0011	XXY	-1.8895	XYY	-0.0006
YYY	3.6052	XXZ	-0.0022	XYZ	0.0000

```
       YYZ      -0.0021    XZZ      -0.0004    YZZ      -0.3290
       ZZZ      -0.0180
    Hexadecapole Moments (Debye-Ang^3)
      XXXX    -194.3823   XXXY       0.0001   XXYY     -57.1554
      XYYY       0.0003   YYYY    -152.8500   XXXZ      -0.0023
      XXYZ      -0.0001   XYYZ      -0.0009   YYYZ       0.0467
      XXZZ     -39.4107   XYZZ      -0.0001   YYZZ     -26.9598
      XZZZ      -0.0022   YZZZ       0.0134   ZZZZ     -35.5778
 ---------------------------------------------------------------
 Calculating analytic gradient of the SCF energy
 Gradient of SCF Energy
           1           2           3           4           5
6
    1   0.0000047   0.0000308   0.0000049   0.0000012   0.0000013
0.0000021
    2   0.0000076   0.0000180
0.0000020  -0.0000123  -0.0000303  -0.0000046
    3  -0.0000015   0.0000083  -0.0000141
0.0000140  -0.0000027  -0.0000103
           7           8           9          10
    1  -0.0000362  -0.0000048  -0.0000013  -0.0000027
    2   0.0000203   0.0000015  -0.0000105   0.0000085
    3   0.0000096  -0.0000138   0.0000115  -0.0000009
 Max gradient component =       3.621E-05
 RMS gradient           =       1.344E-05
 Gradient time:  CPU 0.44 s  wall 0.43 s
 Geometry Optimization Parameters
   NAtoms,    NIC,     NZ,  NCons,   NDum,   NFix, NCnnct, MaxDiis
       10      56       0       0       0       0       0       0

 Cartesian Hessian Update
 Hessian Updated using BFGS Update


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES **
   Searching for a Minimum

   Optimization Cycle:   3

                      Coordinates (Angstroms)
     ATOM                X              Y              Z
      1  H         2.1449253542   -0.0631099035    0.0018681857
      2  C         1.2921345557    0.6180544913   -0.0000941459
      3  H         1.3456873768    1.2709933373    0.8804766405
      4  H         1.3468864705    1.2670105261   -0.8835578787
      5  C         0.0000195544   -0.1738127406    0.0004077407
      6  O         0.0000459372   -1.4153034080    0.0007815543
      7  C        -1.2921253132    0.6180245485   -0.0001679677
      8  H        -1.3457185301    1.2709964802    0.8803751408
```

```
     9  H        -1.3468665092    1.2669397045   -0.8836678165
    10  H        -2.1448914963   -0.0631656358    0.0018007469
   Point Group: c1    Number of degrees of freedom:    24


   Energy is   -193.099779474

 Hessian Updated using BFGS Update

 21 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.006970    0.007145    0.028895    0.072874    0.073157
0.073573
     0.073744    0.143517    0.159995    0.165997    0.248582
0.249998
     0.307313    0.308163    0.336486    0.339409    0.339455
0.339811
     0.345744    0.346570    0.864487

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda =   0.00000000
 Step Taken.  Stepsize is  0.001229

                           Maximum     Tolerance    Cnvgd?
        Gradient           0.000056      0.000300     YES
        Displacement       0.000768      0.001200     YES
        Energy change     -0.000003      0.000001      NO


                    Distance Matrix (Angstroms)
             H (  1)   C (  2)   H (  3)   H (  4)   C (  5)   O (  6)
  C (  2)  1.091440
  H (  3)  1.786215  1.097544
  H (  4)  1.786076  1.097565  1.764039
  C (  5)  2.147761  1.515459  2.161668  2.161346
  O (  6)  2.535535  2.409157  3.130624  3.129032  1.241491
  C (  7)  3.503893  2.584260  2.856564  2.857612  1.515469  2.409176
  H (  8)  3.838777  2.856541  2.691406  3.218944  2.161672  3.130651
  H (  9)  3.840028  2.857636  3.219017  2.693753  2.161356  3.129034
  H ( 10)  4.289817  3.503885  3.838775  3.840018  2.147764  2.535554
             C (  7)   H (  8)   H (  9)
  H (  8)  1.097543
  H (  9)  1.097570  1.764048
  H ( 10)  1.091437  1.786214  1.786079

 Final energy is   -193.09977947448709
```

```
 ****************************
 **  OPTIMIZATION CONVERGED  **
 ****************************

                     Coordinates (Angstroms)
    ATOM                X               Y               Z
     1  H         2.1449253542   -0.0631099035    0.0018681857
     2  C         1.2921345557    0.6180544913   -0.0000941459
     3  H         1.3456873768    1.2709933373    0.8804766405
     4  H         1.3468864705    1.2670105261   -0.8835578787
     5  C         0.0000195544   -0.1738127406    0.0004077407
     6  O         0.0000459372   -1.4153034080    0.0007815543
     7  C        -1.2921253132    0.6180245485   -0.0001679677
     8  H        -1.3457185301    1.2709964802    0.8803751408
     9  H        -1.3468665092    1.2669397045   -0.8836678165
    10  H        -2.1448914963   -0.0631656358    0.0018007469

Z-matrix Print:
$molecule
0 1
C
O  1 1.241491
C  1 1.515459 2 121.500660
H  3 1.091440 1 109.882036 2 -0.107800 0
H  3 1.097544 1 110.621473 2 -120.969914 0
H  3 1.097565 1 110.594578 2 120.719110 0
C  1 1.515469 2 121.501540 3 179.973362 0
H  7 1.091437 1 109.881721 2 0.110876 0
H  7 1.097543 1 110.621176 2 120.972720 0
H  7 1.097570 1 110.594397 2 -120.716006 0
$end


 -----------------------------------------------------------------

                   Orbital Energies (a.u.)
 -----------------------------------------------------------------

 Alpha MOs
 -- Occupied --
-19.139 -10.284 -10.189 -10.189  -1.047  -0.775  -0.717  -0.535
 -0.464  -0.463  -0.449  -0.408  -0.390  -0.382  -0.345  -0.247
 -- Virtual --
 -0.023   0.085   0.136   0.145   0.157   0.169   0.177   0.195
  0.285   0.319   0.507   0.540   0.581   0.591   0.597   0.686
  0.709   0.716   0.793   0.808   0.869   0.937   0.950   0.951
  0.954   0.978   0.995   1.032   1.150   1.246   1.445   1.785
 -----------------------------------------------------------------
```

Ground-State Mulliken Net Atomic Charges

Atom		Charge (a.u.)
1	H	0.174376
2	C	-0.472638
3	H	0.159727
4	H	0.159833
5	C	0.362179
6	O	-0.404775
7	C	-0.472636
8	H	0.159725
9	H	0.159834
10	H	0.174376

Sum of atomic charges = -0.000000

Cartesian Multipole Moments

Charge (ESU x 10^10)
0.0000

Dipole Moment (Debye)

X	-0.0001	Y	3.1676	Z	-0.0025
Tot	3.1676				

Quadrupole Moments (Debye-Ang)

XX	-23.4213	XY	0.0002	YY	-28.9958
XZ	0.0000	YZ	0.0017	ZZ	-24.0796

Octopole Moments (Debye-Ang^2)

XXX	-0.0011	XXY	-1.8895	XYY	-0.0006
YYY	3.6052	XXZ	-0.0022	XYZ	0.0000
YYZ	-0.0021	XZZ	-0.0004	YZZ	-0.3290
ZZZ	-0.0180				

Hexadecapole Moments (Debye-Ang^3)

XXXX	-194.3823	XXXY	0.0001	XXYY	-57.1554
XYYY	0.0003	YYYY	-152.8500	XXXZ	-0.0023
XXYZ	-0.0001	XYYZ	-0.0009	YYYZ	0.0467
XXZZ	-39.4107	XYZZ	-0.0001	YYZZ	-26.9598
XZZZ	-0.0022	YZZZ	0.0134	ZZZZ	-35.5778

Archival summary:
1\1\clab-01\OPT\ProcedureUnspecified\6-31G\136\christia
\MonJun312:26:082019MonJun312:26:082019\0
\\#,OPT,ProcedureUnspecified,6-31G,\\0,1\C\O,1,1.24149
\C,1,1.51546,2,121.501\H,3,1.09144,1,109.882,2,-0.1078,0
\H,3,1.09754,1,110.621,2,-120.97,0\H,3,1.09757,1,110.595,2,120.719,0
\C,1,1.51547,2,121.502,3,179.973,0\H,7,1.09144,1,109.882,2,0.110876,0
\H,7,1.09754,1,110.621,2,120.973,0\H,7,1.09757,1,110.594,2,-120.716,0
\\\@

```
 Total job time:  8.92s(wall), 8.93s(cpu)
 Mon Jun  3 12:26:08 2019

        ************************************************************
        *                                                          *
        *  Thank you very much for using Q-Chem.  Have a nice day.  *
        *                                                          *
        ************************************************************


0 sent ACK to 0
now end server 0 ...

User input: 2 of 4

Process 0 of 1 is on clab-01 - thread support 0
initial socket setup ...start
initial socket setup ...done
now start server 0 ...
Q-Chem Developer Version!
                  Welcome to Q-Chem
     A Quantum Leap Into The Future Of Chemistry


 Q-Chem 5.1, Q-Chem, Inc., Pleasanton, CA (2018)

 Yihan Shao,  Zhengting Gan,  E. Epifanovsky,  A. T. B. Gilbert,  M.
Wormit,
 J. Kussmann,  A. W. Lange,  A. Behn,  Jia Deng,  Xintian Feng,  D.
Ghosh,
 M. Goldey,  P. R. Horn,  L. D. Jacobson,  I. Kaliman,  T. Kus,  A.
Landau,
 Jie Liu,  E. I. Proynov,  R. M. Richard,  R. P. Steele,  E. J.
Sundstrom,
 H. L. Woodcock III,  P. M. Zimmerman,  D. Zuev,  B. Albrecht,  E.
Alguire,
 S. A. Baeppler,  D. Barton,  Z. Benda,  Y. A. Bernard,  E. J.
Berquist,
 K. B. Bravaya,  H. Burton,  D. Casanova,  Chun-Min Chang,  Yunqing
Chen,
 A. Chien,  K. D. Closser,  M. P. Coons,  S. Coriani,  S. Dasgupta,
 A. L. Dempwolff,  M. Diedenhofen,  Hainam Do,  R. G. Edgar,  Po-Tung
Fang,
 S. Faraji,  S. Fatehi,  Qingguo Feng,  K. D. Fenk,  J. Fosso-Tande,
 Qinghui Ge,  A. Ghysels,  G. Gidofalvi,  J. Gomes,  J. Gonthier,  A.
Gunina,
 D. Hait,  M. W. D. Hanson-Heine,  P. H. P. Harbach,  A. W. Hauser,
 J. E. Herr,  E. G. Hohenstein,  Z. C. Holden,  Kerwin Hui,  B. C.
```

Huynh,
T.-C. Jagau, Hyunjun Ji, B. Kaduk, K. Khistyaev, Jaehoon Kim,
P. Klunzinger, K. Koh, D. Kosenkov, L. Koulias, T. Kowalczyk,
C. M. Krauter, A. Kunitsa, Ka Un Lao, A. Laurent, K. V. Lawler,
Joonho Lee, D. Lefrancois, S. Lehtola, D. S. Levine, Yi-Pei Li,
You-Sheng Lin, Fenglai Liu, E. Livshits, A. Luenser, P. Manohar,
E. Mansoor, S. F. Manzer, Shan-Ping Mao, Yuezhi Mao, N. Mardirossian,
A. V. Marenich, T. Markovich, L. A. Martinez-Martinez, S. A. Maurer,
N. J. Mayhall, S. C. McKenzie, J.-M. Mewes, A. F. Morrison,
J. W. Mullinax, K. Nanda, T. S. Nguyen-Beck, R. Olivares-Amaya,
J. A. Parkhill, T. M. Perrine, F. Plasser, P. Pokhilko, S. Prager,
A. Prociuk, E. Ramos, D. R. Rehn, F. Rob, M. Schneider, N. Sergueev,
S. M. Sharada, S. Sharma, D. W. Small, T. Stauch, T. Stein,
Yu-Chuan Su, A. J. W. Thom, A. Tkatchenko, T. Tsuchimochi, N. M. Tubman,
L. Vogt, M. L. Vidal, O. Vydrov, M. A. Watson, J. Wenzel,
M. de Wergifosse, T. A. Wesolowski, A. White, J. Witte, A. Yamada,
Jun Yang, K. Yao, S. Yeganeh, S. R. Yost, Zhi-Qiang You, A. Zech,
Igor Ying Zhang, Xing Zhang, Yan Zhao, Ying Zhu, B. R. Brooks,
G. K. L. Chan, C. J. Cramer, M. S. Gordon, W. J. Hehre, A. Klamt,
M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Aspuru-Guzik, R. Baer,
A. T. Bell, N. A. Besley, Jeng-Da Chai, A. E. DePrince, III,
R. A. DiStasio Jr., A. Dreuw, B. D. Dunietz, T. R. Furlani,
Chao-Ping Hsu, Yousung Jung, Jing Kong, D. S. Lambrecht, WanZhen Liang,
C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik,
T. Van Voorhis, J. M. Herbert, A. I. Krylov, P. M. W. Gill, M. Head-Gordon

Contributors to earlier versions of Q-Chem not listed above:
R. D. Adamson, B. Austin, J. Baker, G. J. O. Beran, K. Brandhorst,
S. T. Brown, E. F. C. Byrd, A. K. Chakraborty, C.-L. Cheng,
Siu Hung Chien, D. M. Chipman, D. L. Crittenden, H. Dachsel,
R. J. Doerksen, A. D. Dutoi, L. Fusti-Molnar, W. A. Goddard III,
A. Golubeva-Zadorozhnaya, S. R. Gwaltney, G. Hawkins, A. Heyden,
S. Hirata, G. Kedziora, F. J. Keil, C. Kelley, Jihan Kim, R. A. King,
R. Z. Khaliullin, P. P. Korambath, W. Kurlancheek, A. M. Lee, M. S. Lee,
S. V. Levchenko, Ching Yeh Lin, D. Liotard, R. C. Lochan, I. Lotan,

```
 P. E. Maslen,  N. Nair,  D. P. O'Neill,  D. Neuhauser,  E.
Neuscamman,
 C. M. Oana,  R. Olson,  B. Peters,  R. Peverati,  P. A. Pieniazek,
 Y. M. Rhee,  J. Ritchie,  M. A. Rohrdanz,  E. Rosta,  N. J. Russ,
 H. F. Schaefer III,  N. E. Schultz,  N. Shenvi,  A. C. Simmonett,  A.
Sodt,
 D. Stuck,  K. S. Thanthiriwatte,  V. Vanovschi,  Tao Wang,  A.
Warshel,
 C. F. Williams,  Q. Wu,  X. Xu,  W. Zhang

 Please cite Q-Chem as follows:
 Y. Shao et al., Mol. Phys. 113, 184-215 (2015)
 DOI: 10.1080/00268976.2014.952696

 Q-Chem 5.1.1 for Intel X86 EM64T Linux

 Parts of Q-Chem use Armadillo 8.300.2 (Tropical Shenanigans).
 http://arma.sourceforge.net/

 Q-Chem begins on Mon Jun  3 12:26:08 2019

Host:
0

     Scratch files written to /home/christian/scratch/qchem24662//
 Parallel job on  1  processors
The previous job contains 0 fragments, simply inherited here
Input Ideriv = 2
Curr. Ideriv = -1
Max.  Ideriv = 2

Checking the input file for inconsistencies...   ...done.

---------------------------------------------------------------
User input:
---------------------------------------------------------------

$comment
Job 2
$end

$molecule
read
$end

$rem
   BASIS  =  6-31G
   GUI  =  2
   JOB_TYPE  =  Frequency
```

```
   METHOD  =  B3LYP
   SCF_CONVERGENCE  =  8
$end


-------------------------------------------------------------
 -------------------------------------------------------------
            Standard Nuclear Orientation (Angstroms)
    I     Atom           X                Y                Z
 -------------------------------------------------------------
    1      H       2.1449083583    -0.0631181859     0.0016384995
    2      C       1.2921115973     0.6180396587     0.0000245948
    3      H       1.3456840060     1.2705600766     0.8809042986
    4      H       1.3468325525     1.2674162910    -0.8831319491
    5      C       0.0000034775    -0.1738389442     0.0001868959
    6      O       0.0000406363    -1.4153296486    -0.0000297726
    7      C      -1.2921482723     0.6179873070     0.0000248490
    8      H      -1.3457219026     1.2705398932     0.8808799625
    9      H      -1.3469204285     1.2673221268    -0.8831646912
   10      H      -2.1449084917    -0.0632111427     0.0016940224
 -------------------------------------------------------------
 Molecular Point Group                C1    NOp =  1
 Largest Abelian Subgroup             C1    NOp =  1
 Nuclear Repulsion Energy =   118.4697303982 hartrees
 There are       16 alpha and       16 beta electrons
 Requested basis set is 6-31G
 There are 24 shells and 48 basis functions

 Total QAlloc Memory Limit   2000 MB
 Mega-Array Size       188 MB
 MEM_STATIC part       192 MB

                      Distance Matrix (Angstroms)
             H (  1)   C (  2)   H (  3)   H (  4)   C (  5)   O (  6)
   C (  2)  1.091440
   H (  3)  1.786215  1.097544
   H (  4)  1.786076  1.097565  1.764039
   C (  5)  2.147761  1.515459  2.161668  2.161346
   O (  6)  2.535535  2.409157  3.130624  3.129032  1.241491
   C (  7)  3.503893  2.584260  2.856564  2.857612  1.515469  2.409176
   H (  8)  3.838777  2.856541  2.691406  3.218944  2.161672  3.130651
   H (  9)  3.840028  2.857636  3.219017  2.693753  2.161356  3.129034
   H ( 10)  4.289817  3.503885  3.838775  3.840018  2.147764  2.535554
             C (  7)   H (  8)   H (  9)
   H (  8)  1.097543
   H (  9)  1.097570  1.764048
   H ( 10)  1.091437  1.786214  1.786079

 A cutoff of  1.0D-11 yielded    297 shell pairs
```

```
 There are      1221 function pairs
 Smallest overlap matrix eigenvalue = 7.67E-03
 Guess from superposition of atomic densities
 Warning:  Energy on first SCF cycle will be non-variational
 SAD guess density has 32.000000 electrons

 ----------------------------------------------------------------------
--
  General SCF calculation program by
  Eric Jon Sundstrom, Paul Horn, Yuezhi Mao, Dmitri Zuev, Alec White,
  David Stuck, Shaama M.S., Shane Yost, Joonho Lee, David Small,
  Daniel Levine, Susi Lehtola, Hugh Burton, Evgeny Epifanovsky
 ----------------------------------------------------------------------
--
 Exchange:     0.2000 Hartree-Fock + 0.0800 Slater + 0.7200 B88
 Correlation:  0.1900 VWN1RPA + 0.8100 LYP
 Using SG-1 standard quadrature grid
 A restricted SCF calculation will be
 performed using DIIS
 SCF converges when DIIS error is below 1.0e-08
 ---------------------------------------
  Cycle       Energy         DIIS error
 ---------------------------------------
    1    -193.6138083830      1.31e-01
    2    -192.9649838087      2.22e-02
    3    -192.7102813546      3.99e-02
    4    -193.0799315982      8.49e-03
    5    -193.0995652985      9.45e-04
    6    -193.0997576328      2.72e-04
    7    -193.0997784689      6.30e-05
    8    -193.0997794623      7.61e-06
    9    -193.0997794752      1.07e-06
   10    -193.0997794755      7.17e-08
   11    -193.0997794755      6.25e-09  Convergence criterion met
 ---------------------------------------
 SCF time:   CPU 2.83s  wall 3.00s
 SCF   energy in the final basis set =     -193.0997794755
 Total energy in the final basis set =     -193.0997794755

 ---------------------------------------------------------------

                    Orbital Energies (a.u.)
 ---------------------------------------------------------------

 Alpha MOs
 -- Occupied --
-19.139 -10.284 -10.189 -10.189  -1.047  -0.775  -0.717  -0.535
 -0.464  -0.463  -0.449  -0.408  -0.390  -0.382  -0.345  -0.247
 -- Virtual --
```

```
-0.023   0.085   0.136   0.145   0.157   0.169   0.177   0.195
 0.285   0.319   0.507   0.540   0.581   0.591   0.597   0.686
 0.709   0.716   0.793   0.808   0.869   0.937   0.950   0.951
 0.954   0.978   0.995   1.032   1.150   1.246   1.445   1.785
-----------------------------------------------------------------

         Ground-State Mulliken Net Atomic Charges

    Atom                  Charge (a.u.)
 ---------------------------------------
     1 H                     0.174376
     2 C                    -0.472638
     3 H                     0.159727
     4 H                     0.159833
     5 C                     0.362179
     6 O                    -0.404775
     7 C                    -0.472636
     8 H                     0.159725
     9 H                     0.159834
    10 H                     0.174376
 ---------------------------------------
 Sum of atomic charges =    -0.000000

-----------------------------------------------------------------------
                    Cartesian Multipole Moments
-----------------------------------------------------------------------
   Charge (ESU x 10^10)
                0.0000
   Dipole Moment (Debye)
        X      -0.0001      Y       3.1676      Z      -0.0010
      Tot       3.1676
   Quadrupole Moments (Debye-Ang)
       XX     -23.4213     XY       0.0001     YY     -28.9960
       XZ       0.0000     YZ      -0.0011     ZZ     -24.0796
   Octopole Moments (Debye-Ang^2)
      XXX       0.0002    XXY      -1.8889    XYY       -0.0002
      YYY       3.6074    XXZ       0.0002    XYZ        0.0001
      YYZ       0.0040    XZZ       0.0000    YZZ       -0.3284
      ZZZ      -0.0085
   Hexadecapole Moments (Debye-Ang^3)
     XXXX    -194.3823   XXXY       0.0000   XXYY      -57.1553
     XYYY       0.0001   YYYY    -152.8505   XXXZ       -0.0001
     XXYZ      -0.0082   XYYZ       0.0000   YYYZ        0.0120
     XXZZ     -39.4107   XYZZ      -0.0002   YYZZ      -26.9598
     XZZZ       0.0002   YZZZ      -0.0080   ZZZZ      -35.5778
-----------------------------------------------------------------------
Calculating MO derivatives via CPSCF
  1         3          30      0.249576    0.089725
  2         3          30      0.011962    0.003966
```

```
   3         4          29      0.000441    0.000142
   4        32           1      0.000005    0.000005
   5        33           0      0.000000    0.000000    Roots
Converged
 Time for AOints: 0.2 s (CPU) 0.2 s (wall)
 ------------------------------------------------------------------------
---------
                      AOints        : Timing summary (seconds)
 ------------------------------------------------------------------------
---------
     job step          cpu (% of tot)      sys (% of tot)     wall (%
of tot)
 ------------------------------------------------------------------------
---------
  cpscf_lag         0.1788E+02 (50.2)   0.1210E-03 (23.0)   0.1788E+02
(50.2)
  iterzp            0.1754E+02 (49.3)   0.4050E-03 (77.0)   0.1754E+02
(49.3)
  make_fx           0.0000E+00 ( 0.0)   0.0000E+00 ( 0.0)   0.0000E+00
( 0.0)
  AOints            0.1653E+00 ( 0.5)   0.0000E+00 ( 0.0)   0.1653E+00
( 0.5)
 ------------------------------------------------------------------------
---------
   Grand Totals     0.3559E+02          0.5260E-03          0.3559E+02
 ------------------------------------------------------------------------
---------
 Calculating analytic Hessian of the SCF energy
 Polarizability Matrix (a.u.)
            1           2           3
    1 -34.6976663   0.0002428  -0.0000293
    2   0.0002428 -39.3479008   0.0017504
    3  -0.0000293   0.0017504 -26.0658141

 Direct stationary perturbation theory relativistic correction:

 rels  =       0.056284105590
 relv  =      -0.242301386056
 rel2e =       0.092815396310
 E_rel =      -0.093201884155

 Hessian of the SCF Energy
            1           2           3           4           5
6
    1   0.2351219  -0.1464050   0.0003525  -0.2136366
0.1317840  -0.0003269
    2  -0.1464050   0.1702755  -0.0002845   0.1376683  -0.1599326
0.0002476
    3   0.0003525  -0.0002845   0.0492975  -0.0003313
```

```
0.0002380  -0.0509325
    4  -0.2136366   0.1376683  -0.0003313   0.5144740  -0.0684959
0.0001071
    5   0.1317840  -0.1599326   0.0002380  -0.0684959   0.5609212
0.0000859
    6  -0.0003269   0.0002476  -0.0509325   0.0001071   0.0000859
0.5277317
    7   0.0022853   0.0145789
0.0221907  -0.0512220  -0.0056637  -0.0126428

8  -0.0026438  -0.0110013  -0.0171933  -0.0045713  -0.1352871  -0.1281
820
    9  -0.0007258   0.0019699
0.0007688  -0.0098444  -0.1256974  -0.2136239
   10   0.0023076   0.0145169  -0.0222440  -0.0512046  -0.0058156
0.0128999
   11  -0.0026563  -0.0109588   0.0172425  -0.0047036  -0.1343571
0.1278747
   12   0.0007380  -0.0019065   0.0006830   0.0100637
0.1253813  -0.2144530
   13  -0.0282853  -0.0187352
0.0000265  -0.1758928  -0.0268478  -0.0000206
   14   0.0241700   0.0109811
0.0000026  -0.0314832  -0.0978889  -0.0000078
   15  -0.0000520  -0.0000362  -0.0009551
0.0000006  -0.0000046  -0.0908682
   16   0.0061005   0.0017363  -0.0000003
0.0058658  -0.0423453  -0.0000153
   17   0.0002265
0.0020939  -0.0000077  -0.0148864  -0.0454650  -0.0000002
   18   0.0000100   0.0000031  -0.0011314  -0.0000050   0.0000136
0.0250044
   19  -0.0034192  -0.0024809   0.0000033  -0.0250358
0.0150166  -0.0000088
   20  -0.0051263  -0.0018140   0.0000004  -0.0150181
0.0136847  -0.0000193
   21   0.0000072   0.0000041   0.0013447   0.0000090  -0.0000196
0.0166264
   22   0.0004502  -0.0000481  -0.0003712
0.0000355  -0.0013794  -0.0025683
   23  -0.0000671  -0.0000658   0.0003556  -0.0004954   0.0000690
0.0009389
   24   0.0001379   0.0001487   0.0002010
0.0001153  -0.0001044  -0.0004140
   25   0.0004497  -0.0000465   0.0003726   0.0000362  -0.0013791
0.0025829
   26  -0.0000667  -0.0000676  -0.0003548  -0.0004952
0.0000694  -0.0009421
   27  -0.0001396  -0.0001474   0.0002020  -0.0001117
```

```
0.0001067  -0.0004156
   28  -0.0013740  -0.0007847   0.0000013  -0.0034196
0.0051262  -0.0000072
   29   0.0007847   0.0004895   0.0000012   0.0024809  -0.0018137
0.0000042
   30  -0.0000013   0.0000012   0.0005219  -0.0000033   0.0000006
0.0013447
            7           8           9          10          11
12
    1   0.0022853  -0.0026438  -0.0007258   0.0023076  -0.0026563
0.0007380
    2   0.0145789  -0.0110013   0.0019699
0.0145169  -0.0109588  -0.0019065
    3   0.0221907  -0.0171933   0.0007688  -0.0222440   0.0172425
0.0006830
    4  -0.0512220  -0.0045713  -0.0098444  -0.0512046  -0.0047036
0.0100637
    5  -0.0056637  -0.1352871  -0.1256974  -0.0058156  -0.1343571
0.1253813
    6  -0.0126428  -0.1281820  -0.2136239   0.0128999
0.1278747  -0.2144530
    7   0.0510372   0.0087078   0.0100272   0.0004336   0.0015290
0.0013604
    8   0.0087078   0.1490797   0.1389815   0.0015002   0.0114799
0.0177258
    9   0.0100272   0.1389815
0.2350875  -0.0013372  -0.0178472  -0.0233683
   10   0.0004336   0.0015002  -0.0013372   0.0510383
0.0088609  -0.0103032
   11   0.0015290   0.0114799  -0.0178472   0.0088609
0.1480792  -0.1386460
   12   0.0013604   0.0177258  -0.0233683  -0.0103032  -0.1386460
0.2360153
   13   0.0015938   0.0006230   0.0023227   0.0015344
0.0005682  -0.0023083
   14  -0.0178378  -0.0141022
0.0010912  -0.0177672  -0.0140716  -0.0010569
   15  -0.0268611  -0.0147742   0.0020865   0.0269287   0.0148402
0.0020753
   16  -0.0033142  -0.0042330  -0.0001106  -0.0032947  -0.0042145
0.0001200
   17  -0.0026876  -0.0009441
0.0013942  -0.0026658  -0.0009411  -0.0013954
   18   0.0030349
0.0018244  -0.0011418  -0.0030385  -0.0018464  -0.0011427
   19   0.0000354   0.0004954  -0.0001153   0.0000362   0.0004952
0.0001116
   20   0.0013793   0.0000690  -0.0001046   0.0013793   0.0000696
0.0001065
```

```
   21   0.0025682
0.0009391  -0.0004141  -0.0025828  -0.0009421  -0.0004155
   22  -0.0015708  -0.0002715  -0.0000140   0.0002717   0.0003254
0.0000628
   23   0.0002714   0.0007547   0.0001931  -0.0003261   0.0000171
0.0001300
   24   0.0000140   0.0001931   0.0005169
0.0000647  -0.0001295  -0.0001128
   25   0.0002717   0.0003262  -0.0000647  -0.0015723  -0.0002711
0.0000152
   26  -0.0003254   0.0000171  -0.0001295   0.0002710
0.0007503  -0.0001913
   27  -0.0000628   0.0001300  -0.0001127  -0.0000152  -0.0001913
0.0005168
   28   0.0004501   0.0000671  -0.0001380   0.0004498   0.0000667
0.0001396
   29   0.0000482  -0.0000657   0.0001487
0.0000465  -0.0000676  -0.0001474
   30   0.0003713   0.0003556   0.0002010  -0.0003725  -0.0003548
0.0002020
           13          14          15          16          17
18
    1  -0.0282853   0.0241700  -0.0000520   0.0061005   0.0002265
0.0000100
    2  -0.0187352   0.0109811  -0.0000362   0.0017363   0.0020939
0.0000031
    3   0.0000265
0.0000026  -0.0009551  -0.0000003  -0.0000077  -0.0011314
    4  -0.1758928  -0.0314832   0.0000006
0.0058658  -0.0148864  -0.0000050
    5  -0.0268478  -0.0978889  -0.0000046  -0.0423453  -0.0454650
0.0000136
    6  -0.0000206  -0.0000078  -0.0908682  -0.0000153  -0.0000002
0.0250044
    7   0.0015938  -0.0178378  -0.0268611  -0.0033142  -0.0026876
0.0030349
    8   0.0006230  -0.0141022  -0.0147742  -0.0042330  -0.0009441
0.0018244
    9   0.0023227   0.0010912   0.0020865  -0.0001106
0.0013942  -0.0011418
   10   0.0015344  -0.0177672
0.0269287  -0.0032947  -0.0026658  -0.0030385
   11   0.0005682  -0.0140716
0.0148402  -0.0042145  -0.0009411  -0.0018464
   12  -0.0023083  -0.0010569   0.0020753
0.0001200  -0.0013954  -0.0011427
   13   0.5065375  -0.0000045  -0.0000004  -0.1044431   0.0000146
0.0000002
   14  -0.0000045   0.8895641   0.0000441
```

```
0.0000160  -0.6594084  -0.0001020
   15  -0.0000004   0.0000441   0.2397002
0.0000001  -0.0000945  -0.0643770
   16  -0.1044431   0.0000160   0.0000001
0.0937313  -0.0000167  -0.0000001
   17   0.0000146  -0.6594084  -0.0000945  -0.0000167   0.7499148
0.0001127
   18   0.0000002  -0.0001020  -0.0643770  -0.0000001   0.0001127
0.0212010
   19  -0.1758859   0.0314725  -0.0000007   0.0058636   0.0148885
0.0000053
   20   0.0268380  -0.0978832  -0.0000049   0.0423464  -0.0454595
0.0000141
   21   0.0000216  -0.0000087  -0.0908684   0.0000156   0.0000002
0.0250034
   22   0.0015938   0.0178397   0.0268610  -0.0033149
0.0026877  -0.0030350
   23  -0.0006230  -0.0141019  -0.0147721   0.0042331  -0.0009437
0.0018239
   24  -0.0023227   0.0010912   0.0020863   0.0001105
0.0013941  -0.0011418
   25   0.0015327   0.0177663  -0.0269297  -0.0032948   0.0026654
0.0030385
   26  -0.0005669  -0.0140700   0.0148395
0.0042140  -0.0009407  -0.0018465
   27   0.0023080  -0.0010566
0.0020754  -0.0001200  -0.0013954  -0.0011427
   28  -0.0282851  -0.0241718   0.0000535
0.0061006  -0.0002262  -0.0000103
   29   0.0187335   0.0109810  -0.0000373  -0.0017363   0.0020939
0.0000032
   30  -0.0000270   0.0000030  -0.0009551
0.0000002  -0.0000080  -0.0011314
          19          20          21          22          23
24
    1  -0.0034192  -0.0051263   0.0000072   0.0004502  -0.0000671
0.0001379
    2  -0.0024809  -0.0018140   0.0000041  -0.0000481  -0.0000658
0.0001487
    3   0.0000033   0.0000004   0.0013447  -0.0003712   0.0003556
0.0002010
    4  -0.0250358  -0.0150181   0.0000090   0.0000355  -0.0004954
0.0001153
    5   0.0150166   0.0136847  -0.0000196  -0.0013794
0.0000690  -0.0001044
    6  -0.0000088  -0.0000193   0.0166264  -0.0025683
0.0009389  -0.0004140
    7   0.0000354   0.0013793   0.0025682  -0.0015708   0.0002714
0.0000140
```

```
    8   0.0004954   0.0000690   0.0009391  -0.0002715   0.0007547
0.0001931
    9  -0.0001153  -0.0001046  -0.0004141  -0.0000140   0.0001931
0.0005169
   10   0.0000362   0.0013793  -0.0025828   0.0002717  -0.0003261
0.0000647
   11   0.0004952   0.0000696  -0.0009421   0.0003254
0.0000171  -0.0001295
   12   0.0001116   0.0001065  -0.0004155   0.0000628
0.0001300  -0.0001128
   13  -0.1758859   0.0268380   0.0000216
0.0015938  -0.0006230  -0.0023227
   14   0.0314725  -0.0978832  -0.0000087   0.0178397  -0.0141019
0.0010912
   15  -0.0000007  -0.0000049  -0.0908684   0.0268610  -0.0147721
0.0020863
   16   0.0058636   0.0423464   0.0000156  -0.0033149   0.0042331
0.0001105
   17   0.0148885  -0.0454595   0.0000002   0.0026877  -0.0009437
0.0013941
   18   0.0000053   0.0000141   0.0250034  -0.0030350
0.0018239  -0.0011418
   19   0.5144607   0.0685063  -0.0001096  -0.0512221   0.0045713
0.0098447
   20   0.0685063   0.5609219   0.0000900
0.0056637  -0.1352978  -0.1257010
   21  -0.0001096   0.0000900   0.5277304
0.0126432  -0.1281851  -0.2136156
   22  -0.0512221   0.0056637   0.0126432
0.0510375  -0.0087081  -0.0100273
   23   0.0045713  -0.1352978  -0.1281851  -0.0087081   0.1490910
0.1389855
   24   0.0098447  -0.1257010  -0.2136156  -0.0100273   0.1389855
0.2350775
   25  -0.0512058   0.0058221  -0.0129101   0.0004337  -0.0015001
0.0013374
   26   0.0047097  -0.1343428   0.1278660  -0.0015300
0.0114798  -0.0178484
   27  -0.0100729   0.1253725  -0.2144597  -0.0013617
0.0177242  -0.0233678
   28  -0.2136271  -0.1317906   0.0003377   0.0022853   0.0026440
0.0007256
   29  -0.1376747  -0.1599479   0.0002561  -0.0145792  -0.0110025
0.0019708
   30   0.0003424   0.0002464  -0.0509317  -0.0221894  -0.0171939
0.0007701
          25          26          27          28          29
30
    1   0.0004497  -0.0000667  -0.0001396  -0.0013740
```

```
0.0007847  -0.0000013
    2  -0.0000465  -0.0000676  -0.0001474  -0.0007847   0.0004895
0.0000012
    3   0.0003726  -0.0003548   0.0002020   0.0000013   0.0000012
0.0005219
    4   0.0000362  -0.0004952  -0.0001117  -0.0034196
0.0024809  -0.0000033
    5  -0.0013791   0.0000694   0.0001067   0.0051262  -0.0018137
0.0000006
    6   0.0025829  -0.0009421  -0.0004156  -0.0000072   0.0000042
0.0013447
    7   0.0002717  -0.0003254  -0.0000628   0.0004501   0.0000482
0.0003713
    8   0.0003262   0.0000171   0.0001300   0.0000671  -0.0000657
0.0003556
    9  -0.0000647  -0.0001295  -0.0001127  -0.0001380   0.0001487
0.0002010
   10  -0.0015723   0.0002710  -0.0000152   0.0004498
0.0000465  -0.0003725
   11  -0.0002711   0.0007503  -0.0001913
0.0000667  -0.0000676  -0.0003548
   12   0.0000152  -0.0001913   0.0005168   0.0001396  -0.0001474
0.0002020
   13   0.0015327  -0.0005669   0.0023080  -0.0282851
0.0187335  -0.0000270
   14   0.0177663  -0.0140700  -0.0010566  -0.0241718   0.0109810
0.0000030
   15  -0.0269297   0.0148395   0.0020754
0.0000535  -0.0000373  -0.0009551
   16  -0.0032948   0.0042140  -0.0001200   0.0061006  -0.0017363
0.0000002
   17   0.0026654  -0.0009407  -0.0013954  -0.0002262
0.0020939  -0.0000080
   18   0.0030385  -0.0018465  -0.0011427  -0.0000103
0.0000032  -0.0011314
   19  -0.0512058   0.0047097  -0.0100729  -0.2136271  -0.1376747
0.0003424
   20   0.0058221  -0.1343428   0.1253725  -0.1317906  -0.1599479
0.0002464
   21  -0.0129101   0.1278660  -0.2144597   0.0003377
0.0002561  -0.0509317
   22   0.0004337  -0.0015300  -0.0013617
0.0022853  -0.0145792  -0.0221894
   23  -0.0015001   0.0114798   0.0177242
0.0026440  -0.0110025  -0.0171939
   24   0.0013374  -0.0178484  -0.0233678   0.0007256   0.0019708
0.0007701
   25   0.0510400  -0.0088679   0.0103140   0.0023088  -0.0145153
0.0222438
```

```
   26  -0.0088679   0.1480631  -0.1386370   0.0026574  -0.0109587
0.0172440
   27   0.0103140  -0.1386370   0.2360228  -0.0007381  -0.0019055
0.0006816
   28   0.0023088   0.0026574  -0.0007381   0.2351112
0.1464118  -0.0003642
   29  -0.0145153  -0.0109587  -0.0019055   0.1464118
0.1702916  -0.0002939
   30   0.0222438   0.0172440   0.0006816  -0.0003642  -0.0002939
0.0492968
 Gradient time:  CPU 43.26 s  wall 43.26 s

*********************************************************************
 **
**
 **                        VIBRATIONAL ANALYSIS
**
 **                        --------------------
**
 **
**
 **        VIBRATIONAL FREQUENCIES (CM**-1) AND NORMAL MODES
**
 **     FORCE CONSTANTS (mDYN/ANGSTROM) AND REDUCED MASSES (AMU)
**
 **                   INFRARED INTENSITIES (KM/MOL)
**
 **
**

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


 Mode:                    1                         2                         3
 Frequency:          88.33                    152.60                    388.02
 Force Cnst:        0.0047                    0.0154                    0.1966
 Red. Mass:         1.0181                    1.1258                    2.2159
 IR Active:            YES                       YES                       YES
 IR Intens:          0.000                     0.188                     1.416
 Raman Active:         YES                       YES                       YES
                X      Y      Z        X      Y      Z        X      Y
Z
 H          -0.000  0.001  0.349   -0.000  0.000
0.410   -0.066 -0.381 -0.000
 C          -0.000  0.000 -0.022    0.000 -0.000  0.036
0.156 -0.100 -0.000
 H          -0.148  0.321 -0.253   -0.160  0.317 -0.194    0.366 -0.126
0.006
 H           0.149 -0.322 -0.251    0.161 -0.318 -0.192
```

```
0.365 -0.126 -0.005
 C         -0.000  0.000  0.000    0.000  0.000  0.024   -0.000
0.131 -0.000
 O          0.000  0.000 -0.000   -0.000  0.000 -0.075   -0.000  0.132
0.000
 C         -0.000 -0.000  0.022   -0.000 -0.000
0.036   -0.156 -0.100 -0.000
 H         -0.148 -0.321  0.253    0.160  0.317 -0.194   -0.366 -0.126
0.006
 H          0.149  0.322
0.251   -0.161 -0.318 -0.192   -0.365 -0.126 -0.005
 H         -0.000 -0.001 -0.349    0.000  0.000  0.410
0.066 -0.381 -0.000
 TransDip   0.000 -0.000 -0.000   -0.000 -0.000 -0.014    0.000 -0.038
0.000

 Mode:                 4                      5                      6
 Frequency:       499.33                 533.13                 796.50
 Force Cnst:      0.3110                 0.6140                 1.4532
 Red. Mass:       2.1170                 3.6668                 3.8879
 IR Active:          YES                    YES                    YES
 IR Intens:        0.100                 15.058                  0.331
 Raman Active:       YES                    YES                    YES
               X      Y      Z        X      Y      Z        X      Y
Z
 H          0.001 -0.000 -0.309   -0.339 -0.440 -0.000   -0.414 -0.301
0.000
 C          0.000 -0.000 -0.026   -0.122 -0.168  0.000   -0.279 -0.142
0.000
 H          0.363  0.142 -0.160    0.080 -0.195
0.006   -0.183 -0.151 -0.003
 H         -0.364 -0.143 -0.160    0.079 -0.195 -0.006   -0.183 -0.152
0.003
 C          0.000  0.000  0.293   -0.145 -0.000  0.000   -0.000
0.137 -0.000
 O         -0.000  0.000 -0.101    0.314  0.000 -0.000    0.000  0.186
0.000
 C         -0.000 -0.000 -0.026   -0.122  0.168 -0.000    0.279 -0.142
0.000
 H         -0.363  0.142 -0.160    0.080  0.195 -0.006
0.183 -0.151 -0.003
 H          0.364 -0.143 -0.160    0.079  0.195  0.006    0.184 -0.152
0.003
 H         -0.001 -0.000 -0.309   -0.339  0.440  0.000    0.414 -0.301
0.000
 TransDip   0.000 -0.000  0.010   -0.124 -0.000  0.000   -0.000
0.018 -0.000

 Mode:                 7                      8                      9
```

```
 Frequency:       931.88                934.17                1114.98
 Force Cnst:      0.8129                0.6221                 1.1412
 Red. Mass:       1.5889                1.2100                 1.5580
 IR Active:          YES                   YES                    YES
 IR Intens:        5.196                 0.020                  0.033
 Raman Active:       YES                   YES                    YES
               X      Y      Z        X      Y      Z        X      Y
Z
 H         -0.286 -0.276  0.015   -0.015 -0.015 -0.216    0.405  0.332
0.000
 C          0.031  0.134 -0.007    0.002  0.007  0.095
0.064 -0.111 -0.000
 H          0.364  0.028  0.048    0.407  0.242 -0.118   -0.315
0.001 -0.054
 H          0.418  0.062 -0.030   -0.366 -0.238 -0.122   -0.313  0.002
0.054
 C         -0.119 -0.000  0.000   -0.006  0.000 -0.000    0.000  0.019
0.000
 O         -0.021 -0.000 -0.000   -0.001  0.000  0.000   -0.000
0.110 -0.000
 C          0.031 -0.134  0.007
0.002 -0.007 -0.095   -0.064 -0.111 -0.000
 H          0.364 -0.028 -0.048    0.407 -0.242  0.118    0.315
0.001 -0.054
 H          0.418 -0.062  0.030   -0.366  0.238  0.122    0.313  0.002
0.054
 H         -0.286  0.276 -0.015   -0.015  0.015  0.216   -0.405  0.332
0.000
 TransDip  -0.073 -0.000 -0.000   -0.005 -0.000 -0.000    0.000 -0.006
0.000

 Mode:                10                    11                    12
 Frequency:       1151.50               1270.72               1433.35
 Force Cnst:       1.4546                3.2509                1.5330
 Red. Mass:        1.8619                3.4170                1.2664
 IR Active:          YES                   YES                    YES
 IR Intens:        5.972                91.754                49.973
 Raman Active:       YES                   YES                    YES
               X      Y      Z        X      Y      Z        X      Y
Z
 H         -0.001 -0.000  0.265   -0.447 -0.357 -0.000    0.199
0.298 -0.001
 C         -0.000  0.000 -0.124   -0.142  0.036  0.000   -0.091 -0.054
0.000
 H         -0.332 -0.268  0.114    0.074 -0.134  0.091    0.359
0.153 -0.166
 H          0.334  0.268  0.113    0.074 -0.135 -0.091    0.359  0.154
0.165
 C          0.000 -0.000  0.212    0.414  0.000 -0.000
```

```
0.033 -0.000 -0.000
 O         -0.000 -0.000 -0.035   -0.060  0.000  0.000   -0.003
0.000 -0.000
 C          0.000  0.000 -0.124   -0.142 -0.036 -0.000   -0.091
0.054 -0.000
 H          0.332 -0.268  0.114    0.074  0.134 -0.091    0.359 -0.153
0.166
 H         -0.334  0.268  0.113    0.074  0.135  0.091
0.359 -0.154 -0.166
 H          0.001 -0.000  0.265   -0.447  0.357  0.000    0.199 -0.298
0.001
 TransDip   0.000 -0.000  0.078    0.307  0.000  0.000    0.226 -0.000
0.000

 Mode:                 13                    14                    15
 Frequency:       1440.25               1505.73               1511.70
 Force Cnst:       1.4787                1.3954                1.4681
 Red. Mass:        1.2099                1.0446                1.0904
 IR Active:           YES                   YES                   YES
 IR Intens:        24.908                 1.710                32.634
 Raman Active:        YES                   YES                   YES
               X      Y      Z        X      Y      Z        X      Y
Z
 H          0.208  0.292 -0.001    0.171  0.253 -0.000   -0.167 -0.255
0.001
 C         -0.077 -0.056  0.000   -0.027  0.028 -0.000    0.035 -0.028
0.000
 H          0.339  0.180 -0.184    0.107 -0.351  0.260   -0.143
0.344 -0.251
 H          0.339  0.181  0.184    0.107 -0.352 -0.259   -0.144  0.345
0.250
 C          0.000  0.009  0.000   -0.018 -0.000  0.000   -0.000  0.037
0.000
 O         -0.000 -0.005 -0.000    0.005  0.000 -0.000
0.000 -0.039 -0.000
 C          0.077 -0.056  0.000   -0.027 -0.028  0.000   -0.035 -0.028
0.000
 H         -0.339  0.180 -0.184    0.107  0.351 -0.260    0.143
0.344 -0.251
 H         -0.339  0.181  0.183    0.107  0.352  0.259    0.144  0.345
0.250
 H         -0.207  0.292 -0.001    0.171 -0.253  0.000    0.167 -0.255
0.001
 TransDip   0.000  0.160 -0.000    0.042  0.000 -0.000   -0.000
0.183 -0.000

 Mode:                 16                    17                    18
 Frequency:       1514.16               1533.78               1730.57
 Force Cnst:       1.4245                1.4487                13.1971
```

```
 Red. Mass:       1.0546                1.0452                7.4791
 IR Active:          YES                   YES                   YES
 IR Intens:        0.000                28.017               113.800
 Raman Active:       YES                   YES                   YES
               X      Y      Z        X      Y      Z        X      Y
Z
 H          0.000 -0.001 -0.524   -0.000  0.001  0.508    0.189
0.238 -0.000
 C          0.000  0.000
0.046   -0.000 -0.000 -0.036   -0.008 -0.045 -0.000
 H         -0.307  0.125 -0.047    0.328 -0.106  0.039   -0.107 -0.202
0.132
 H          0.306 -0.125 -0.047   -0.327  0.106
0.038   -0.107 -0.202 -0.132
 C         -0.000 -0.000 -0.000   -0.000 -0.000 -0.028   -0.000  0.623
0.000
 O          0.000  0.000  0.000    0.000 -0.000  0.001
0.000 -0.379 -0.000
 C          0.000 -0.000 -0.046    0.000 -0.000 -0.036
0.008 -0.045 -0.000
 H         -0.307 -0.125  0.047   -0.328 -0.106  0.039    0.107 -0.202
0.132
 H          0.306  0.125  0.047    0.327  0.106  0.038
0.107 -0.202 -0.132
 H          0.000  0.001  0.524    0.000  0.001  0.508   -0.189
0.238 -0.000
 TransDip  -0.000 -0.000  0.000    0.000  0.000  0.170   -0.000
0.342 -0.000

 Mode:              19                    20                    21
 Frequency:      3042.01               3048.13               3104.36
 Force Cnst:       5.6564                5.6783                6.2294
 Red. Mass:        1.0375                1.0373                1.0971
 IR Active:          YES                   YES                   YES
 IR Intens:        1.659                 7.934                 0.000
 Raman Active:       YES                   YES                   YES
               X      Y      Z        X      Y      Z        X      Y
Z
 H          0.205 -0.176  0.000   -0.212  0.179 -0.000   -0.001  0.001
0.019
 C         -0.021 -0.030  0.000    0.021  0.030 -0.000    0.000  0.000
0.064
 H          0.017  0.265
0.376   -0.017 -0.265 -0.375   -0.022 -0.304 -0.393
 H          0.018  0.265 -0.378   -0.017 -0.264  0.377    0.023
0.303 -0.394
 C          0.002  0.000 -0.000   -0.000  0.000 -0.000   -0.000
0.000 -0.000
 O         -0.000 -0.000 -0.000    0.000 -0.001 -0.000   -0.000
```

```
0.000 -0.000
 C         -0.021  0.030 -0.000   -0.021  0.030 -0.000
0.000 -0.000 -0.064
 H          0.017 -0.266 -0.377    0.016 -0.264 -0.374   -0.022  0.305
0.394
 H          0.018 -0.265  0.379    0.017 -0.264  0.376    0.023 -0.303
0.394
 H          0.205  0.176 -0.000    0.211
0.179 -0.000   -0.001 -0.001 -0.019
 TransDip  -0.041  0.000 -0.000    0.000  0.090 -0.000
0.000 -0.000 -0.000

 Mode:                 22                    23                    24
 Frequency:       3111.25               3170.88               3171.98
 Force Cnst:       6.2579                6.5093                6.5164
 Red. Mass:        1.0973                1.0988                1.0992
 IR Active:           YES                   YES                   YES
 IR Intens:        24.191                13.324                 7.833
 Raman Active:        YES                   YES                   YES
               X      Y      Z        X      Y      Z        X      Y
Z
 H          0.001 -0.001 -0.017    0.517 -0.413  0.001   -0.503
0.403 -0.001
 C         -0.000 -0.000 -0.064   -0.040  0.051 -0.000    0.040 -0.050
0.000
 H          0.023  0.305  0.394   -0.016 -0.101 -0.155    0.017  0.102
0.156
 H         -0.023 -0.303  0.394   -0.016 -0.100  0.155    0.017
0.101 -0.156
 C         -0.000  0.000 -0.001   -0.001  0.000 -0.000   -0.000 -0.004
0.000
 O          0.000 -0.000 -0.000    0.000 -0.000 -0.000    0.000
0.001 -0.000
 C          0.000 -0.000 -0.064   -0.040 -0.050  0.000   -0.041 -0.051
0.000
 H         -0.022  0.305  0.393   -0.015  0.098  0.152   -0.017  0.104
0.160
 H          0.023 -0.303  0.393   -0.016  0.097 -0.151   -0.017
0.103 -0.159
 H         -0.001 -0.001 -0.017    0.506  0.405 -0.001    0.514
0.412 -0.001
 TransDip   0.000 -0.000 -0.158   -0.117
0.001 -0.000   -0.001 -0.090 -0.000

 STANDARD THERMODYNAMIC QUANTITIES AT   298.15 K  AND     1.00 ATM

   This Molecule has  0 Imaginary Frequencies
   Zero point vibrational energy:       53.150 kcal/mol
```

```
  Atom    1 Element H  Has Mass    1.00783
  Atom    2 Element C  Has Mass   12.00000
  Atom    3 Element H  Has Mass    1.00783
  Atom    4 Element H  Has Mass    1.00783
  Atom    5 Element C  Has Mass   12.00000
  Atom    6 Element O  Has Mass   15.99491
  Atom    7 Element C  Has Mass   12.00000
  Atom    8 Element H  Has Mass    1.00783
  Atom    9 Element H  Has Mass    1.00783
  Atom   10 Element H  Has Mass    1.00783
  Molecular Mass:    58.041890 amu
  Principal axes and moments of inertia in amu*Bohr^2:
                           1           2           3
   Eigenvalues --      181.37801   213.50209   372.48084
         X               1.00000     0.00002     0.00000
         Y              -0.00002     1.00000    -0.00001
         Z              -0.00000     0.00001     1.00000
  Rotational Symmetry Number is   1
  The Molecule is an Asymmetric Top
  Translational Enthalpy:        0.889 kcal/mol
  Rotational Enthalpy:           0.889 kcal/mol
  Vibrational Enthalpy:         54.661 kcal/mol
  gas constant (RT):             0.592 kcal/mol
  Translational Entropy:        38.096  cal/mol.K
  Rotational Entropy:           24.182  cal/mol.K
  Vibrational Entropy:           9.258  cal/mol.K

  Total Enthalpy:               57.031 kcal/mol
  Total Entropy:                71.536  cal/mol.K


=========================================================================

 STANDARD THERMODYNAMIC QUANTITIES FOR ANHARMONIC VIBRATION -- TOSH

  Zero point vibrational energy: ************ kcal/mol

  Vibrational Enthalpy:       Infinity kcal/mol
  Vibrational Entropy:             NaN  cal/mol.K

  Total Enthalpy:             Infinity kcal/mol
  Total Entropy:                   NaN  cal/mol.K


=========================================================================

 STANDARD THERMODYNAMIC QUANTITIES FOR ANHARMONIC VIBRATION -- VPT2

  Zero point vibrational energy: ************ kcal/mol
```

```
   Vibrational Enthalpy:       Infinity kcal/mol
   Vibrational Entropy:             NaN  cal/mol.K

   Total Enthalpy:             Infinity kcal/mol
   Total Entropy:                   NaN  cal/mol.K


===============================================================================

Archival summary:
1\1\clab-01\FREQ\ProcedureUnspecified\6-31G\136\christia
\MonJun312:26:542019MonJun312:26:542019\0
\\#,FREQ,ProcedureUnspecified,6-31G,\\0,1\C\O,1,1.24149
\C,1,1.51546,2,121.501\H,3,1.09144,1,109.882,2,-0.1078,0
\H,3,1.09754,1,110.621,2,-120.97,0\H,3,1.09757,1,110.595,2,120.719,0
\C,1,1.51547,2,121.502,3,179.973,0\H,7,1.09144,1,109.882,2,0.110876,0
\H,7,1.09754,1,110.621,2,120.973,0\H,7,1.09757,1,110.594,2,-120.716,0
\\\@

 Total job time:  46.13s(wall), 46.12s(cpu)
 Mon Jun  3 12:26:54 2019

        ************************************************************
        *                                                          *
        *  Thank you very much for using Q-Chem.  Have a nice day.  *
        *                                                          *
        ************************************************************


0 sent ACK to 0
now end server 0 ...

User input: 3 of 4

Process 0 of 1 is on clab-01 - thread support 0
initial socket setup ...start
initial socket setup ...done
now start server 0 ...
Q-Chem Developer Version!
                  Welcome to Q-Chem
     A Quantum Leap Into The Future Of Chemistry


 Q-Chem 5.1, Q-Chem, Inc., Pleasanton, CA (2018)

 Yihan Shao,  Zhengting Gan,  E. Epifanovsky,  A. T. B. Gilbert,  M.
Wormit,
 J. Kussmann,  A. W. Lange,  A. Behn,  Jia Deng,  Xintian Feng,  D.
```

Ghosh,
M. Goldey, P. R. Horn, L. D. Jacobson, I. Kaliman, T. Kus, A. Landau,
Jie Liu, E. I. Proynov, R. M. Richard, R. P. Steele, E. J. Sundstrom,
H. L. Woodcock III, P. M. Zimmerman, D. Zuev, B. Albrecht, E. Alguire,
S. A. Baeppler, D. Barton, Z. Benda, Y. A. Bernard, E. J. Berquist,
K. B. Bravaya, H. Burton, D. Casanova, Chun-Min Chang, Yunqing Chen,
A. Chien, K. D. Closser, M. P. Coons, S. Coriani, S. Dasgupta,
A. L. Dempwolff, M. Diedenhofen, Hainam Do, R. G. Edgar, Po-Tung Fang,
S. Faraji, S. Fatehi, Qingguo Feng, K. D. Fenk, J. Fosso-Tande,
Qinghui Ge, A. Ghysels, G. Gidofalvi, J. Gomes, J. Gonthier, A. Gunina,
D. Hait, M. W. D. Hanson-Heine, P. H. P. Harbach, A. W. Hauser,
J. E. Herr, E. G. Hohenstein, Z. C. Holden, Kerwin Hui, B. C. Huynh,
T.-C. Jagau, Hyunjun Ji, B. Kaduk, K. Khistyaev, Jaehoon Kim,
P. Klunzinger, K. Koh, D. Kosenkov, L. Koulias, T. Kowalczyk,
C. M. Krauter, A. Kunitsa, Ka Un Lao, A. Laurent, K. V. Lawler,
Joonho Lee, D. Lefrancois, S. Lehtola, D. S. Levine, Yi-Pei Li,
You-Sheng Lin, Fenglai Liu, E. Livshits, A. Luenser, P. Manohar,
E. Mansoor, S. F. Manzer, Shan-Ping Mao, Yuezhi Mao, N. Mardirossian,
A. V. Marenich, T. Markovich, L. A. Martinez-Martinez, S. A. Maurer,
N. J. Mayhall, S. C. McKenzie, J.-M. Mewes, A. F. Morrison,
J. W. Mullinax, K. Nanda, T. S. Nguyen-Beck, R. Olivares-Amaya,
J. A. Parkhill, T. M. Perrine, F. Plasser, P. Pokhilko, S. Prager,
A. Prociuk, E. Ramos, D. R. Rehn, F. Rob, M. Schneider, N. Sergueev,
S. M. Sharada, S. Sharma, D. W. Small, T. Stauch, T. Stein,
Yu-Chuan Su, A. J. W. Thom, A. Tkatchenko, T. Tsuchimochi, N. M. Tubman,
L. Vogt, M. L. Vidal, O. Vydrov, M. A. Watson, J. Wenzel,
M. de Wergifosse, T. A. Wesolowski, A. White, J. Witte, A. Yamada,
Jun Yang, K. Yao, S. Yeganeh, S. R. Yost, Zhi-Qiang You, A. Zech,
Igor Ying Zhang, Xing Zhang, Yan Zhao, Ying Zhu, B. R. Brooks,
G. K. L. Chan, C. J. Cramer, M. S. Gordon, W. J. Hehre, A. Klamt,
M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Aspuru-Guzik, R. Baer,
A. T. Bell, N. A. Besley, Jeng-Da Chai, A. E. DePrince, III,
R. A. DiStasio Jr., A. Dreuw, B. D. Dunietz, T. R. Furlani,

Chao-Ping Hsu, Yousung Jung, Jing Kong, D. S. Lambrecht, WanZhen Liang,
C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik,
T. Van Voorhis, J. M. Herbert, A. I. Krylov, P. M. W. Gill, M. Head-Gordon

Contributors to earlier versions of Q-Chem not listed above:
R. D. Adamson, B. Austin, J. Baker, G. J. O. Beran, K. Brandhorst,
S. T. Brown, E. F. C. Byrd, A. K. Chakraborty, C.-L. Cheng,
Siu Hung Chien, D. M. Chipman, D. L. Crittenden, H. Dachsel,
R. J. Doerksen, A. D. Dutoi, L. Fusti-Molnar, W. A. Goddard III,
A. Golubeva-Zadorozhnaya, S. R. Gwaltney, G. Hawkins, A. Heyden,
S. Hirata, G. Kedziora, F. J. Keil, C. Kelley, Jihan Kim, R. A. King,
R. Z. Khaliullin, P. P. Korambath, W. Kurlancheek, A. M. Lee, M. S. Lee,
S. V. Levchenko, Ching Yeh Lin, D. Liotard, R. C. Lochan, I. Lotan,
P. E. Maslen, N. Nair, D. P. O'Neill, D. Neuhauser, E. Neuscamman,
C. M. Oana, R. Olson, B. Peters, R. Peverati, P. A. Pieniazek,
Y. M. Rhee, J. Ritchie, M. A. Rohrdanz, E. Rosta, N. J. Russ,
H. F. Schaefer III, N. E. Schultz, N. Shenvi, A. C. Simmonett, A. Sodt,
D. Stuck, K. S. Thanthiriwatte, V. Vanovschi, Tao Wang, A. Warshel,
C. F. Williams, Q. Wu, X. Xu, W. Zhang

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Q-Chem 5.1.1 for Intel X86 EM64T Linux

Parts of Q-Chem use Armadillo 8.300.2 (Tropical Shenanigans).
http://arma.sourceforge.net/

Q-Chem begins on Mon Jun 3 12:26:55 2019

Host:
0

Scratch files written to /home/christian/scratch/qchem24662//
Parallel job on 1 processors
The previous job contains 0 fragments, simply inherited here
Input Ideriv = 2
Curr. Ideriv = -1
Max. Ideriv = 2

```
Checking the input file for inconsistencies...   ...done.

-----------------------------------------------------------------
User input:
-----------------------------------------------------------------

$comment
Job 3
$end

$molecule
read
$end

$rem
   BASIS  =  6-31G
   CIS_MAX_CYCLES  =  50
   CIS_N_ROOTS  =  5
   CIS_TRIPLETS  =  0
   GUI  =  2
   JOB_TYPE  =  SP
   METHOD  =  CIS
   RPA  =  0
   SCF_CONVERGENCE  =  8
$end


-----------------------------------------------------------------
 ---------------------------------------------------------------
            Standard Nuclear Orientation (Angstroms)
    I     Atom           X                Y                Z
 ---------------------------------------------------------------
    1      H       2.1449083583    -0.0631181859     0.0016384995
    2      C       1.2921115973     0.6180396587     0.0000245948
    3      H       1.3456840060     1.2705600766     0.8809042986
    4      H       1.3468325525     1.2674162910    -0.8831319491
    5      C       0.0000034775    -0.1738389442     0.0001868959
    6      O       0.0000406363    -1.4153296486    -0.0000297726
    7      C      -1.2921482723     0.6179873070     0.0000248490
    8      H      -1.3457219026     1.2705398932     0.8808799625
    9      H      -1.3469204285     1.2673221268    -0.8831646912
   10      H      -2.1449084917    -0.0632111427     0.0016940224
 ---------------------------------------------------------------
 Molecular Point Group                 C1    NOp =  1
 Largest Abelian Subgroup              C1    NOp =  1
 Nuclear Repulsion Energy =   118.4697303982 hartrees
 There are       16 alpha and       16 beta electrons
 Requested basis set is 6-31G
```

```
 There are 24 shells and 48 basis functions

 Total QAlloc Memory Limit   2000 MB
 Mega-Array Size       188 MB
 MEM_STATIC part       192 MB

                      Distance Matrix (Angstroms)
            H (  1)   C (  2)   H (  3)   H (  4)   C (  5)   O (  6)
  C (  2)  1.091440
  H (  3)  1.786215  1.097544
  H (  4)  1.786076  1.097565  1.764039
  C (  5)  2.147761  1.515459  2.161668  2.161346
  O (  6)  2.535535  2.409157  3.130624  3.129032  1.241491
  C (  7)  3.503893  2.584260  2.856564  2.857612  1.515469  2.409176
  H (  8)  3.838777  2.856541  2.691406  3.218944  2.161672  3.130651
  H (  9)  3.840028  2.857636  3.219017  2.693753  2.161356  3.129034
  H ( 10)  4.289817  3.503885  3.838775  3.840018  2.147764  2.535554
            C (  7)   H (  8)   H (  9)
  H (  8)  1.097543
  H (  9)  1.097570  1.764048
  H ( 10)  1.091437  1.786214  1.786079

 A cutoff of  1.0D-11 yielded    297 shell pairs
 There are      1221 function pairs
 Smallest overlap matrix eigenvalue = 7.67E-03

 Scale SEOQF with 1.000000e-01/1.000000e+00/1.000000e+00

 Standard Electronic Orientation quadrupole field applied
 Nucleus-field energy     =     0.0000000174 hartrees
 Guess from superposition of atomic densities
 Warning:  Energy on first SCF cycle will be non-variational
 SAD guess density has 32.000000 electrons

 ------------------------------------------------------------------------
--
  General SCF calculation program by
  Eric Jon Sundstrom, Paul Horn, Yuezhi Mao, Dmitri Zuev, Alec White,
  David Stuck, Shaama M.S., Shane Yost, Joonho Lee, David Small,
  Daniel Levine, Susi Lehtola, Hugh Burton, Evgeny Epifanovsky
 ------------------------------------------------------------------------
--
 Hartree-Fock
 A restricted SCF calculation will be
 performed using DIIS
 SCF converges when DIIS error is below 1.0e-08
 ---------------------------------------
  Cycle       Energy         DIIS error
 ---------------------------------------
```

```
    1    -192.8342766878      1.39e-01
    2    -191.7635483566      1.83e-02
    3    -191.8169672182      1.59e-02
    4    -191.8716281614      1.46e-03
    5    -191.8732039939      5.74e-04
    6    -191.8734256489      2.57e-04
    7    -191.8734839886      9.10e-05
    8    -191.8734897244      1.54e-05
    9    -191.8734899045      3.57e-06
   10    -191.8734899107      7.39e-07
   11    -191.8734899110      9.46e-08
   12    -191.8734899110      1.87e-08
   13    -191.8734899110      2.43e-09  Convergence criterion met
 ---------------------------------------
 SCF time:   CPU 0.54s  wall 0.00s
 SCF   energy in the final basis set =     -191.8734899110
 Total energy in the final basis set =     -191.8734899110

 Direct RCIS calculation will be performed
 Singlet excitation energies requested
 CIS energy converged when residual is below 10e- 6
 ----------------------------------------------------
 Iter    Rts Conv    Rts Left    Ttl Dev     Max Dev
 ----------------------------------------------------
   1         0           5      0.018899    0.008698
   2         0           5      0.006328    0.002150
   3         0           5      0.002157    0.000641
   4         0           5      0.005604    0.004740
   5         0           5      0.003126    0.002850
   6         1           4      0.000985    0.000884
   7         1           4      0.000363    0.000316
   8         1           4      0.000112    0.000085
   9         3           2      0.000042    0.000026
  10         3           2      0.000014    0.000007
  11         3           2      0.000004    0.000001
  12         5           0      0.000002    0.000001    Roots
Converged
 ----------------------------------------------------

 ----------------------------------------------------
              CIS Excitation Energies
 ----------------------------------------------------

 Excited state   1: excitation energy (eV) =    4.7661
 Total energy for state  1:                 -191.69833865 au
    Multiplicity: Singlet
    Trans. Mom.: -0.0001 X  -0.0000 Y  -0.0000 Z
    Strength   :     0.0000000015
    D( 16) --> V(  1) amplitude =  0.9553
```

```
 Excited state   2: excitation energy (eV) =    9.1955
 Total energy for state  2:                 -191.53555972 au
    Multiplicity: Singlet
    Trans. Mom.: -0.0000 X  -0.0004 Y  -0.0006 Z
    Strength   :     0.0000001168
    D( 10) --> V(  1) amplitude =  0.5362
    D( 13) --> V(  1) amplitude = -0.7905

 Excited state   3: excitation energy (eV) =    9.6890
 Total energy for state  3:                 -191.51742404 au
    Multiplicity: Singlet
    Trans. Mom.: -0.0000 X   1.2269 Y  -0.0008 Z
    Strength   :     0.3573012748
    D( 15) --> V(  1) amplitude =  0.9259

 Excited state   4: excitation energy (eV) =   10.4784
 Total energy for state  4:                 -191.48841742 au
    Multiplicity: Singlet
    Trans. Mom.: -0.0004 X  -0.0000 Y   0.0000 Z
    Strength   :     0.0000000448
    D(  9) --> V(  1) amplitude = -0.5222
    D( 14) --> V(  1) amplitude =  0.8032

 Excited state   5: excitation energy (eV) =   11.5526
 Total energy for state  5:                 -191.44893945 au
    Multiplicity: Singlet
    Trans. Mom.:  0.3091 X  -0.0000 Y   0.0000 Z
    Strength   :     0.0270458100
    D( 16) --> V(  2) amplitude =  0.9263
    D( 16) --> V(  3) amplitude =  0.2395
    D( 16) --> V( 10) amplitude = -0.2143

 -----------------------------------------------------
  SETman timing summary (seconds)
  CPU time                 0.92s
  System time              0.00s
  Wall time                0.85s

 ------------------------------------------------------------------

                     Orbital Energies (a.u.)
 ------------------------------------------------------------------

 Alpha MOs
 -- Occupied --
-20.561 -11.352 -11.243 -11.243  -1.389  -1.049  -0.975  -0.743
 -0.647  -0.631  -0.624  -0.562  -0.555  -0.538  -0.473  -0.415
 -- Virtual --
```

```
 0.143   0.219   0.277   0.287   0.307   0.316   0.327   0.356
 0.454   0.488   0.716   0.760   0.783   0.825   0.826   0.928
 0.957   0.963   1.029   1.044   1.149   1.200   1.211   1.219
 1.232   1.243   1.277   1.334   1.427   1.474   1.693   2.080
 -------------------------------------------------------------

         Ground-State Mulliken Net Atomic Charges

    Atom                  Charge (a.u.)
  ---------------------------------------
     1 H                     0.208828
     2 C                    -0.541408
     3 H                     0.181251
     4 H                     0.181347
     5 C                     0.486474
     6 O                    -0.546514
     7 C                    -0.541405
     8 H                     0.181250
     9 H                     0.181349
    10 H                     0.208828
  ---------------------------------------
  Sum of atomic charges =    -0.000000

 ---------------------------------------------------------------------
                    Cartesian Multipole Moments
 ---------------------------------------------------------------------
    Charge (ESU x 10^10)
                  0.0000
    Dipole Moment (Debye)
         X      -0.0001      Y       3.7200      Z      -0.0007
       Tot       3.7200
    Quadrupole Moments (Debye-Ang)
        XX     -23.5595     XY       0.0002     YY     -30.3731
        XZ       0.0000     YZ      -0.0010     ZZ     -24.5501
    Octopole Moments (Debye-Ang^2)
       XXX       0.0002    XXY      -1.7461    XYY      -0.0002
       YYY       5.4912    XXZ       0.0012    XYZ       0.0001
       YYZ       0.0047    XZZ      -0.0000    YZZ      -0.0064
       ZZZ      -0.0087
    Hexadecapole Moments (Debye-Ang^3)
      XXXX    -194.4540   XXXY       0.0000   XXYY     -57.6698
      XYYY       0.0002   YYYY    -158.5698   XXXZ      -0.0002
      XXYZ      -0.0087   XYYZ      -0.0000   YYYZ       0.0136
      XXZZ     -40.1568   XYZZ      -0.0002   YYZZ     -27.7106
      XZZZ       0.0002   YZZZ      -0.0083   ZZZZ     -36.2794
 ---------------------------------------------------------------------
Archival summary:
1\1\clab-01\SP\HF\6-31G\136\christia
\MonJun312:26:562019MonJun312:26:562019\0\\#,HF,6-31G,\\0,1\C
```

```
\O,1,1.24149\C,1,1.51546,2,121.501\H,3,1.09144,1,109.882,2,-0.1078,0
\H,3,1.09754,1,110.621,2,-120.97,0\H,3,1.09757,1,110.595,2,120.719,0
\C,1,1.51547,2,121.502,3,179.973,0\H,7,1.09144,1,109.882,2,0.110876,0
\H,7,1.09754,1,110.621,2,120.973,0\H,7,1.09757,1,110.594,2,-120.716,0
\\HF=-191.87349\\@

 Total job time:  1.43s(wall), 1.49s(cpu)
 Mon Jun  3 12:26:56 2019

        ************************************************************
        *                                                          *
        *  Thank you very much for using Q-Chem.  Have a nice day.  *
        *                                                          *
        ************************************************************


0 sent ACK to 0
now end server 0 ...

User input: 4 of 4

Process 0 of 1 is on clab-01 - thread support 0
initial socket setup ...start
initial socket setup ...done
now start server 0 ...
Q-Chem Developer Version!
                  Welcome to Q-Chem
     A Quantum Leap Into The Future Of Chemistry


 Q-Chem 5.1, Q-Chem, Inc., Pleasanton, CA (2018)

 Yihan Shao,  Zhengting Gan,  E. Epifanovsky,  A. T. B. Gilbert,  M.
Wormit,
 J. Kussmann,  A. W. Lange,  A. Behn,  Jia Deng,  Xintian Feng,  D.
Ghosh,
 M. Goldey,  P. R. Horn,  L. D. Jacobson,  I. Kaliman,  T. Kus,  A.
Landau,
 Jie Liu,  E. I. Proynov,  R. M. Richard,  R. P. Steele,  E. J.
Sundstrom,
 H. L. Woodcock III,  P. M. Zimmerman,  D. Zuev,  B. Albrecht,  E.
Alguire,
 S. A. Baeppler,  D. Barton,  Z. Benda,  Y. A. Bernard,  E. J.
Berquist,
 K. B. Bravaya,  H. Burton,  D. Casanova,  Chun-Min Chang,  Yunqing
Chen,
 A. Chien,  K. D. Closser,  M. P. Coons,  S. Coriani,  S. Dasgupta,
 A. L. Dempwolff,  M. Diedenhofen,  Hainam Do,  R. G. Edgar,  Po-Tung
Fang,
```

S. Faraji, S. Fatehi, Qingguo Feng, K. D. Fenk, J. Fosso-Tande, Qinghui Ge, A. Ghysels, G. Gidofalvi, J. Gomes, J. Gonthier, A. Gunina, D. Hait, M. W. D. Hanson-Heine, P. H. P. Harbach, A. W. Hauser, J. E. Herr, E. G. Hohenstein, Z. C. Holden, Kerwin Hui, B. C. Huynh, T.-C. Jagau, Hyunjun Ji, B. Kaduk, K. Khistyaev, Jaehoon Kim, P. Klunzinger, K. Koh, D. Kosenkov, L. Koulias, T. Kowalczyk, C. M. Krauter, A. Kunitsa, Ka Un Lao, A. Laurent, K. V. Lawler, Joonho Lee, D. Lefrancois, S. Lehtola, D. S. Levine, Yi-Pei Li, You-Sheng Lin, Fenglai Liu, E. Livshits, A. Luenser, P. Manohar, E. Mansoor, S. F. Manzer, Shan-Ping Mao, Yuezhi Mao, N. Mardirossian, A. V. Marenich, T. Markovich, L. A. Martinez-Martinez, S. A. Maurer, N. J. Mayhall, S. C. McKenzie, J.-M. Mewes, A. F. Morrison, J. W. Mullinax, K. Nanda, T. S. Nguyen-Beck, R. Olivares-Amaya, J. A. Parkhill, T. M. Perrine, F. Plasser, P. Pokhilko, S. Prager, A. Prociuk, E. Ramos, D. R. Rehn, F. Rob, M. Schneider, N. Sergueev, S. M. Sharada, S. Sharma, D. W. Small, T. Stauch, T. Stein, Yu-Chuan Su, A. J. W. Thom, A. Tkatchenko, T. Tsuchimochi, N. M. Tubman, L. Vogt, M. L. Vidal, O. Vydrov, M. A. Watson, J. Wenzel, M. de Wergifosse, T. A. Wesolowski, A. White, J. Witte, A. Yamada, Jun Yang, K. Yao, S. Yeganeh, S. R. Yost, Zhi-Qiang You, A. Zech, Igor Ying Zhang, Xing Zhang, Yan Zhao, Ying Zhu, B. R. Brooks, G. K. L. Chan, C. J. Cramer, M. S. Gordon, W. J. Hehre, A. Klamt, M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Aspuru-Guzik, R. Baer, A. T. Bell, N. A. Besley, Jeng-Da Chai, A. E. DePrince, III, R. A. DiStasio Jr., A. Dreuw, B. D. Dunietz, T. R. Furlani, Chao-Ping Hsu, Yousung Jung, Jing Kong, D. S. Lambrecht, WanZhen Liang, C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik, T. Van Voorhis, J. M. Herbert, A. I. Krylov, P. M. W. Gill, M. Head-Gordon

Contributors to earlier versions of Q-Chem not listed above:
R. D. Adamson, B. Austin, J. Baker, G. J. O. Beran, K. Brandhorst, S. T. Brown, E. F. C. Byrd, A. K. Chakraborty, C.-L. Cheng, Siu Hung Chien, D. M. Chipman, D. L. Crittenden, H. Dachsel, R. J. Doerksen, A. D. Dutoi, L. Fusti-Molnar, W. A. Goddard III, A. Golubeva-Zadorozhnaya, S. R. Gwaltney, G. Hawkins, A. Heyden, S. Hirata, G. Kedziora, F. J. Keil, C. Kelley, Jihan Kim, R. A.

```
King,
 R. Z. Khaliullin,  P. P. Korambath,  W. Kurlancheek,  A. M. Lee,  M.
S. Lee,
 S. V. Levchenko,  Ching Yeh Lin,  D. Liotard,  R. C. Lochan,  I.
Lotan,
 P. E. Maslen,  N. Nair,  D. P. O'Neill,  D. Neuhauser,  E.
Neuscamman,
 C. M. Oana,  R. Olson,  B. Peters,  R. Peverati,  P. A. Pieniazek,
 Y. M. Rhee,  J. Ritchie,  M. A. Rohrdanz,  E. Rosta,  N. J. Russ,
 H. F. Schaefer III,  N. E. Schultz,  N. Shenvi,  A. C. Simmonett,  A.
Sodt,
 D. Stuck,  K. S. Thanthiriwatte,  V. Vanovschi,  Tao Wang,  A.
Warshel,
 C. F. Williams,  Q. Wu,  X. Xu,  W. Zhang

 Please cite Q-Chem as follows:
 Y. Shao et al., Mol. Phys. 113, 184-215 (2015)
 DOI: 10.1080/00268976.2014.952696

 Q-Chem 5.1.1 for Intel X86 EM64T Linux

 Parts of Q-Chem use Armadillo 8.300.2 (Tropical Shenanigans).
 http://arma.sourceforge.net/

 Q-Chem begins on Mon Jun  3 12:26:56 2019

Host:
0

     Scratch files written to /home/christian/scratch/qchem24662//
 Parallel job on  1  processors
The previous job contains 0 fragments, simply inherited here
Input Ideriv = 2
Curr. Ideriv = -1
Max.  Ideriv = 2

Checking the input file for inconsistencies...   ...done.

---------------------------------------------------------------
User input:
---------------------------------------------------------------

$molecule
read
$end

$rem
   BASIS  =  6-31G
   CIS_N_ROOTS  =  5
```

```
   CIS_TRIPLETS  =  0
   EXCHANGE  =  B3LYP
   GUI  =  2
   JOB_TYPE  =  SP
   RPA  =  1
   SCF_CONVERGENCE  =  8
$end

-----------------------------------------------------------------
 -----------------------------------------------------------------
            Standard Nuclear Orientation (Angstroms)
    I     Atom           X                Y                Z
 -----------------------------------------------------------------
    1      H       2.1449083583    -0.0631181859     0.0016384995
    2      C       1.2921115973     0.6180396587     0.0000245948
    3      H       1.3456840060     1.2705600766     0.8809042986
    4      H       1.3468325525     1.2674162910    -0.8831319491
    5      C       0.0000034775    -0.1738389442     0.0001868959
    6      O       0.0000406363    -1.4153296486    -0.0000297726
    7      C      -1.2921482723     0.6179873070     0.0000248490
    8      H      -1.3457219026     1.2705398932     0.8808799625
    9      H      -1.3469204285     1.2673221268    -0.8831646912
   10      H      -2.1449084917    -0.0632111427     0.0016940224
 -----------------------------------------------------------------
 Molecular Point Group                C1    NOp =  1
 Largest Abelian Subgroup             C1    NOp =  1
 Nuclear Repulsion Energy =   118.4697303982 hartrees
 There are       16 alpha and       16 beta electrons
 Requested basis set is 6-31G
 There are 24 shells and 48 basis functions

 Total QAlloc Memory Limit   2000 MB
 Mega-Array Size       188 MB
 MEM_STATIC part       192 MB

                     Distance Matrix (Angstroms)
             H (  1)   C (  2)   H (  3)   H (  4)   C (  5)   O (  6)
   C (  2)  1.091440
   H (  3)  1.786215  1.097544
   H (  4)  1.786076  1.097565  1.764039
   C (  5)  2.147761  1.515459  2.161668  2.161346
   O (  6)  2.535535  2.409157  3.130624  3.129032  1.241491
   C (  7)  3.503893  2.584260  2.856564  2.857612  1.515469  2.409176
   H (  8)  3.838777  2.856541  2.691406  3.218944  2.161672  3.130651
   H (  9)  3.840028  2.857636  3.219017  2.693753  2.161356  3.129034
   H ( 10)  4.289817  3.503885  3.838775  3.840018  2.147764  2.535554
             C (  7)   H (  8)   H (  9)
   H (  8)  1.097543
   H (  9)  1.097570  1.764048
```

```
   H ( 10)  1.091437  1.786214  1.786079

 A cutoff of  1.0D-11 yielded    297 shell pairs
 There are      1221 function pairs
 Smallest overlap matrix eigenvalue = 7.67E-03

 Scale SEOQF with 1.000000e-01/1.000000e+00/1.000000e+00

 Standard Electronic Orientation quadrupole field applied
 Nucleus-field energy     =     0.0000000174 hartrees
 Guess from superposition of atomic densities
 Warning:  Energy on first SCF cycle will be non-variational
 SAD guess density has 32.000000 electrons

 ------------------------------------------------------------------------
--
  General SCF calculation program by
  Eric Jon Sundstrom, Paul Horn, Yuezhi Mao, Dmitri Zuev, Alec White,
  David Stuck, Shaama M.S., Shane Yost, Joonho Lee, David Small,
  Daniel Levine, Susi Lehtola, Hugh Burton, Evgeny Epifanovsky
 ------------------------------------------------------------------------
--
 Exchange:     0.2000 Hartree-Fock + 0.0800 Slater + 0.7200 B88
 Correlation:  0.1900 VWN1RPA + 0.8100 LYP
 Using SG-1 standard quadrature grid
 A restricted SCF calculation will be
 performed using DIIS
 SCF converges when DIIS error is below 1.0e-08
 ---------------------------------------
  Cycle       Energy         DIIS error
 ---------------------------------------
    1    -193.6138083809      1.31e-01
    2    -192.9649838068      2.22e-02
    3    -192.7102813490      3.99e-02
    4    -193.0799315973      8.49e-03
    5    -193.0995652976      9.45e-04
    6    -193.0997576319      2.72e-04
    7    -193.0997784680      6.30e-05
    8    -193.0997794614      7.61e-06
    9    -193.0997794743      1.07e-06
   10    -193.0997794747      7.17e-08
   11    -193.0997794747      6.25e-09  Convergence criterion met
 ---------------------------------------
 SCF time:   CPU 2.98s  wall 3.00s
 SCF   energy in the final basis set =     -193.0997794747
 Total energy in the final basis set =     -193.0997794747

 Direct TDDFT/TDA calculation will be performed
 Exchange:     0.2000 Hartree-Fock + 0.0800 Slater + 0.7200 B88
```

```
 Correlation:  0.1900 VWN1RPA + 0.8100 LYP
 Using SG-1 standard quadrature grid
 Singlet excitation energies requested
 CIS energy converged when residual is below 10e- 6
 ----------------------------------------------------
 Iter    Rts Conv    Rts Left    Ttl Dev     Max Dev
 ----------------------------------------------------
   1         0           5      0.014186    0.010606
   2         0           5      0.007352    0.006424
   3         0           5      0.002245    0.002076
   4         1           4      0.002448    0.002410
   5         2           3      0.000376    0.000371
   6         4           1      0.000076    0.000074
   7         4           1      0.000017    0.000015
   8         4           1      0.000005    0.000004
   9         5           0      0.000002    0.000001    Roots
Converged
 ----------------------------------------------------

 ----------------------------------------------------
         TDDFT/TDA Excitation Energies
 ----------------------------------------------------

 Excited state   1: excitation energy (eV) =    4.1804
 Total energy for state  1:                 -192.94615219 au
    Multiplicity: Singlet
    Trans. Mom.: -0.0001 X  -0.0000 Y   0.0000 Z
    Strength   :     0.0000000004
    D( 16) --> V(  1) amplitude =  0.9973

 Excited state   2: excitation energy (eV) =    8.0530
 Total energy for state  2:                 -192.80383719 au
    Multiplicity: Singlet
    Trans. Mom.:  0.2987 X   0.0000 Y   0.0000 Z
    Strength   :     0.0175998641
    D( 16) --> V(  2) amplitude =  0.9990

 Excited state   3: excitation energy (eV) =    8.3465
 Total energy for state  3:                 -192.79305078 au
    Multiplicity: Singlet
    Trans. Mom.: -0.0006 X  -0.0000 Y   0.0000 Z
    Strength   :     0.0000000767
    D( 14) --> V(  1) amplitude =  0.9920

 Excited state   4: excitation energy (eV) =    8.4636
 Total energy for state  4:                 -192.78874715 au
    Multiplicity: Singlet
    Trans. Mom.:  0.0000 X   0.0005 Y   0.0556 Z
    Strength   :     0.0006418918
```

```
   D( 13) --> V(  1) amplitude =  0.9899

 Excited state   5: excitation energy (eV) =    9.1073
 Total energy for state  5:                 -192.76509155 au
   Multiplicity: Singlet
   Trans. Mom.: -0.0000 X   0.7492 Y  -0.0011 Z
   Strength   :     0.1252414259
   D( 10) --> V(  1) amplitude =  0.2159
   D( 15) --> V(  1) amplitude =  0.7662
   D( 16) --> V(  4) amplitude = -0.5506

 ---------------------------------------------------

 Direct TDDFT calculation will be performed
 Exchange:     0.2000 Hartree-Fock + 0.0800 Slater + 0.7200 B88
 Correlation:  0.1900 VWN1RPA + 0.8100 LYP
 Using SG-1 standard quadrature grid
 ---------------------------------------------------
 Iter    Rts Conv    Rts Left    Ttl Dev     Max Dev
 ---------------------------------------------------
   1         0           5      0.000127    0.000073
   2         0           5      0.000354    0.000249
   3         0           5      0.000263    0.000237
   4         1           4      0.000080    0.000061
   5         1           4      0.000044    0.000036
   6         2           3      0.000012    0.000005
   7         2           3      0.000007    0.000003
   8         3           2      0.000006    0.000003
   9         3           2      0.000007    0.000004
  10         2           3      0.000005    0.000002
  11         4           1      0.000004    0.000002
  12         4           1      0.000003    0.000001
  13         5           0      0.000003    0.000001    Roots
Converged
 ---------------------------------------------------

 ---------------------------------------------------
            TDDFT Excitation Energies
 ---------------------------------------------------

 Excited state   1: excitation energy (eV) =    4.1616
 Total energy for state  1:                 -192.94684510 au
   Multiplicity: Singlet
   Trans. Mom.: -0.0000 X  -0.0000 Y   0.0001 Z
   Strength   :     0.0000000007
   X: D( 16) --> V(  1) amplitude =  0.9982

 Excited state   2: excitation energy (eV) =    8.0499
 Total energy for state  2:                 -192.80395129 au
```

```
   Multiplicity: Singlet
   Trans. Mom.:  0.2916 X  -0.0000 Y   0.0001 Z
   Strength   :     0.0167688723
   X: D( 16) --> V(  2) amplitude =  0.9991

 Excited state   3: excitation energy (eV) =    8.3439
 Total energy for state  3:                 -192.79314725 au
   Multiplicity: Singlet
   Trans. Mom.: -0.0004 X   0.0001 Y   0.0002 Z
   Strength   :     0.0000000435
   X: D( 14) --> V(  1) amplitude =  0.9921

 Excited state   4: excitation energy (eV) =    8.4222
 Total energy for state  4:                 -192.79027080 au
   Multiplicity: Singlet
   Trans. Mom.: -0.0004 X   0.0011 Y   0.0427 Z
   Strength   :     0.0003767315
   X: D( 13) --> V(  1) amplitude =  0.9901

 Excited state   5: excitation energy (eV) =    8.8249
 Total energy for state  5:                 -192.77546930 au
   Multiplicity: Singlet
   Trans. Mom.: -0.0010 X   0.8271 Y  -0.0004 Z
   Strength   :     0.1478979381
   X: D( 15) --> V(  1) amplitude =  0.8898
   X: D( 16) --> V(  4) amplitude = -0.3772

 -----------------------------------------------------
  SETman timing summary (seconds)
  CPU time                11.14s
  System time              0.00s
  Wall time               11.03s

 ------------------------------------------------------------------

                    Orbital Energies (a.u.)
 ------------------------------------------------------------------

 Alpha MOs
 -- Occupied --
-19.139 -10.284 -10.189 -10.189  -1.047  -0.775  -0.717  -0.535
 -0.464  -0.463  -0.449  -0.408  -0.390  -0.382  -0.345  -0.247
 -- Virtual --
 -0.023   0.085   0.136   0.145   0.157   0.169   0.177   0.195
  0.285   0.319   0.507   0.540   0.581   0.591   0.597   0.686
  0.709   0.716   0.793   0.808   0.869   0.937   0.950   0.951
  0.954   0.978   0.995   1.032   1.150   1.246   1.445   1.785
 ------------------------------------------------------------------
```

Ground-State Mulliken Net Atomic Charges

Atom		Charge (a.u.)
1	H	0.174376
2	C	-0.472638
3	H	0.159727
4	H	0.159833
5	C	0.362179
6	O	-0.404775
7	C	-0.472636
8	H	0.159725
9	H	0.159834
10	H	0.174376

Sum of atomic charges = -0.000000

Cartesian Multipole Moments

Charge (ESU x 10^10)
0.0000

Dipole Moment (Debye)

X	-0.0001	Y	3.1676	Z	-0.0010
Tot	3.1676				

Quadrupole Moments (Debye-Ang)

XX	-23.4213	XY	0.0001	YY	-28.9960
XZ	0.0000	YZ	-0.0011	ZZ	-24.0796

Octopole Moments (Debye-Ang^2)

XXX	0.0002	XXY	-1.8889	XYY	-0.0002
YYY	3.6074	XXZ	0.0002	XYZ	0.0001
YYZ	0.0040	XZZ	0.0000	YZZ	-0.3284
ZZZ	-0.0085				

Hexadecapole Moments (Debye-Ang^3)

XXXX	-194.3823	XXXY	0.0000	XXYY	-57.1553
XYYY	0.0001	YYYY	-152.8505	XXXZ	-0.0001
XXYZ	-0.0082	XYYZ	0.0000	YYYZ	0.0120
XXZZ	-39.4107	XYZZ	-0.0002	YYZZ	-26.9598
XZZZ	0.0002	YZZZ	-0.0080	ZZZZ	-35.5778

Archival summary:
1\1\clab-01\SP\ProcedureUnspecified\6-31G\136\christia
\MonJun312:27:102019MonJun312:27:102019\0
\\#,ProcedureUnspecified,6-31G,\\0,1\C\O,1,1.24149
\C,1,1.51546,2,121.501\H,3,1.09144,1,109.882,2,-0.1078,0
\H,3,1.09754,1,110.621,2,-120.97,0\H,3,1.09757,1,110.595,2,120.719,0
\C,1,1.51547,2,121.502,3,179.973,0\H,7,1.09144,1,109.882,2,0.110876,0
\H,7,1.09754,1,110.621,2,120.973,0\H,7,1.09757,1,110.594,2,-120.716,0
\\\@

```
 Total job time:  14.05s(wall), 14.16s(cpu)
 Mon Jun  3 12:27:10 2019

        ************************************************************
        *                                                          *
        *  Thank you very much for using Q-Chem.  Have a nice day.  *
        *                                                          *
        ************************************************************


0 sent ACK to 0
now end server 0 ...
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