View Job 99948: CH3ON, Geometry Optimization - Gaussian

Status

guest
webmo
1:00
unlimited
0 jobs

Summary

- CH3ON
- Job # 99948
- 3/12/2012
- 36.2 sec

Actions

Job Manager
Raw output
All files
Print
Help

Notes

Molecule Viewer Data Viewer

File Edit View Symmetry Help

View Mode - Rotate (drag = rotate XY; alt-drag = rotate Z)

Reset Viewer | New Job Using This Geometry | Export Molecule

Calculated Quantities

Quantity	Value
Route	#N HF/6-31G(d) OPT(NewEstmFC) Geom=Connectivity

Geometry Sequence

Step	Energy
0	-168.875553493
1	-168.911973933
2	-168.924440010
3	-168.913338537
4	-168.928639941
5	-168.929105243
6	-168.930294247
7	-168.930526700
8	-168.930641286
9	-168.930677463
10	-168.930688926
11	-168.930696283
12	-168.930699082
13	-168.930701781
14	-168.930702570
15	-168.930702708
16	-168.930702726
Animation speed	5
Loop	None

Quantity	Value
Stoichiometry	CH_3NO
Symmetry	C1
Basis	6-31G(d)
RHF Energy	-168.930702726 Hartree

Rotational Constants

Constant	Frequency (GHz)	Frequency (cm^{-1})
a	75.6114324	2.52212590351
b	11.6032817	0.38704381616
c	10.0595498	0.33555046271

Dipole Moment: 4.1006 Debye

Partial Charges

Atom	Symbol	Charge
1	C	0.508341
2	O	-0.554663
3	N	-0.884260
4	H	0.388913
5	H	0.398363
6	H	0.143306

Quote

A AA AAA AAAA AAAAA AAAAAA KKKKKKKK AAAAAAA KKKKKKKK AAAAAAAA KKKKKKKK ZZZZZZZZZZZZZZZZZZZZ AAAA AAA KKKKKKKK ZZZZZZZZZZZZZZZZZZZ AAAA AAA KKKKKKKK K ZZZZZZZZZZZZZZZZZZ AAAA AAA KKKKKKKK KKK ZZZZZZZZZZZZZZZZZ AAAA AAA KKKKKKKK KKKKK ZZZZZZZZZZZZZZZZ AAAA AAA KKKKKKKK KKKKKKK ZZZZZZ AAAA AAA KKKKKKKK KKKKKKK ZZZZZZ AAAA AAA KKKKKKKK KKKKKKK ZZZZZZ AAAA AAA KKKKKKKK KKKKKKK ZZZZZZ AAAA AAA KKKKKKKK KKKKKKK ZZZZZZ AAAAAAAAAAAAAAAAAA KKKKKKKK KKKKKKK ZZZZZZ AAAAAAAAAAAAAAAAAAA KKKKKKKK KKKKKKK ZZZZZZ AAAAAAAAAAAAAAAAAAAA KKKKKKKKKKKKKKK ZZZZZZ AAAAAAAAAAAAAAAAAAAAA KKKKKKKKKKKKKK ZZZZZZ AAAAAA AAAAAAAA KKKKKKKKKKKKK ZZZZZZ AAAAAA AAAAAAAA KKKKKKKKKKKK ZZZZZZ AAAAAA AAAAAAAA KKKKKKKKKKK ZZZZZZ AAAAAA AAAAAAAA KKKKKKKKKKKK ZZZZZZ AAAAAA AAAAAAAA KKKKKKKKKKKKK ZZZZZZ AAAAAA AAAAAAAA KKKKKKKKKKKKKK ZZZZZZ AAAAAA AAAAAAAA KKKKKKKKKKKKKKK ZZZZZZ AAAAAA AAAAAAAA KKKKK KKKKKKKKKK ZZZZZZ AAAAAA AAAAAAAA KKKKK KKKKKKKKKK ZZZZZZ AAAAAA KKKKK KKKKKKKKKK ZZZZZZ AAAAAA KKKKK KKKKKKKKKK ZZZZZZ KKKKK KKKKKKKKKK ZZZZZZ KKKKK KKKKKKKKKK ZZZZZZ KKKKK KKKKKKKKKK ZZZZZZ KKKKK KKKKKKKKKK ZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZ KKKKK KKKKKKKKKK ZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZ KKKKK KKKKKKKKKK ZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZ KKKKK KKKKKKKKKK ZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZ KKKKK KKKKKKKKKK ZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZ KKKKK KKKKKKKKKK ZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZ KKKKK KKKKKKKKKK ZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZ KKKKK KKKKKKKKKK ZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZ KKKKK

	KKKKKKKKKK ZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZZ KKKKK KKKKK (J.P.)
Server	buchner.chem.hope.edu (32286)
CPU time	36.2 sec

```
Entering Gaussian System, Link 0=/usr/local/g09/g09
Initial command:
/usr/local/g09/l1.exe /scratch/webmodemo/webmo-4350/99948/Gau-32286.inp -scrdir=/scratch/webmodemo/webmo-4350/99948/
Entering Link 1 = /usr/local/g09/l1.exe PID=     32287.

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

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

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

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

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

                  RESTRICTED RIGHTS LEGEND

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

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


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


Cite this work as:
Gaussian 09, Revision A.02,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

******************************************
Gaussian 09:  AM64L-G09RevA.02 11-Jun-2009
               12-Mar-2012
******************************************
----------------------------------------------
#N HF/6-31G(d) OPT(NewEstmFC) Geom=Connectivity
----------------------------------------------
1/10=7,18=20,19=15,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=1,11=9,16=1,25=1,30=1,71=1/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/29=1/1,2,3,16;
```

```
1/10=7,18=20,19=15/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=1,11=9,16=1,25=1,30=1,71=1/1,2,3;
4/5=5,16=3/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/18=20,19=15/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
-----
CH3ON
-----
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C
O                    1    B1
N                    1    B2       2    A1
H                    3    B3       1    A2       2    D1       0
H                    3    B4       1    A3       2    D2       0
H                    1    B5       2    A4       3    D3       0
      Variables:
 B1                    1.275
 B2                    1.52
 B3                    1.07
 B4                    1.07
 B5                    1.09
 A1                  109.47122
 A2                  109.47122
 A3                  109.47122
 A4                  125.26439
 D1                  180.
 D2                  -60.
 D3                  180.

    3 tetrahedral angles replaced.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.275          estimate D2E/DX2                !
! R2    R(1,3)                  1.52           estimate D2E/DX2                !
! R3    R(1,6)                  1.09           estimate D2E/DX2                !
! R4    R(3,4)                  1.07           estimate D2E/DX2                !
! R5    R(3,5)                  1.07           estimate D2E/DX2                !
! A1    A(2,1,3)              109.4712         estimate D2E/DX2                !
! A2    A(2,1,6)              125.2644         estimate D2E/DX2                !
! A3    A(3,1,6)              125.2644         estimate D2E/DX2                !
! A4    A(1,3,4)              109.4712         estimate D2E/DX2                !
! A5    A(1,3,5)              109.4712         estimate D2E/DX2                !
! A6    A(4,3,5)              109.4712         estimate D2E/DX2                !
! D1    D(2,1,3,4)            180.0            estimate D2E/DX2                !
! D2    D(2,1,3,5)            -60.0            estimate D2E/DX2                !
! D3    D(6,1,3,4)              0.0            estimate D2E/DX2                !
! D4    D(6,1,3,5)            120.0            estimate D2E/DX2                !
--------------------------------------------------------------------------------
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  25 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.000000    0.000000    0.000000
     2          8           0        0.000000    0.000000    1.275000
     3          7           0        1.433070    0.000000   -0.506667
     4          1           0        1.433070    0.000000   -1.576667
     5          1           0        1.937473    0.873651   -0.150000
     6          1           0       -0.889981    0.000000   -0.629312
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.275000   0.000000
    3  N    1.520000   2.286487   0.000000
    4  H    2.130626   3.191503   1.070000   0.000000
    5  H    2.130626   2.558846   1.070000   1.747303   0.000000
    6  H    1.090000   2.102016   2.326286   2.508794   2.997916
                  6
```

```
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                       Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.210884    0.509153    0.038312
     2          8           0       -1.167941   -0.330508   -0.029787
     3          7           0        1.114354   -0.219757   -0.112795
     4          1           0        1.917531    0.484900   -0.055645
     5          1           0        1.216147   -0.940943    0.671061
     6          1           0       -0.325326    1.583486    0.182572
---------------------------------------------------------------------
Rotational constants (GHZ):     51.4283372     11.0936135      9.3482491
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        67.5990534226 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
Petite list used in FoFCou.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.875553493     A.U. after   15 cycles
            Convg  =    0.2286D-08             -V/T =  2.0063

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

           Population analysis using the SCF density.

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

Orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
The electronic state is 1-A.
Alpha  occ. eigenvalues --  -20.56296 -15.60100 -11.38443  -1.35751  -1.15399
Alpha  occ. eigenvalues --   -0.84194  -0.69077  -0.64341  -0.59754  -0.52331
Alpha  occ. eigenvalues --   -0.44091  -0.42112
Alpha virt. eigenvalues --    0.13392   0.21160   0.23903   0.29527   0.37568
Alpha virt. eigenvalues --    0.46551   0.75109   0.78541   0.84991   0.88535
Alpha virt. eigenvalues --    0.93950   1.00683   1.04524   1.10086   1.12177
Alpha virt. eigenvalues --    1.15995   1.17629   1.28815   1.36191   1.43042
Alpha virt. eigenvalues --    1.63652   1.69150   1.76320   1.96204   2.05244
Alpha virt. eigenvalues --    2.12199   2.15827   2.30792   2.36777   2.49459
Alpha virt. eigenvalues --    2.52468   2.66622   2.83424   2.90923   3.09888
Alpha virt. eigenvalues --    3.24894   4.09083   4.12626   4.52522
         Condensed to atoms (all electrons):
              1          2          3          4          5          6
    1  C    4.426677   0.514739   0.301983  -0.023281  -0.014927   0.364835
    2  O    0.514739   8.134826  -0.102565   0.004151   0.000763  -0.036612
    3  N    0.301983  -0.102565   7.088392   0.291656   0.306258  -0.056186
    4  H   -0.023281   0.004151   0.291656   0.416691  -0.018929   0.002313
    5  H   -0.014927   0.000763   0.306258  -0.018929   0.345852   0.002380
    6  H    0.364835  -0.036612  -0.056186   0.002313   0.002380   0.514407
```

```
Mulliken atomic charges:
             1
    1  C    0.429975
    2  O   -0.515302
    3  N   -0.829538
    4  H    0.327399
    5  H    0.378603
    6  H    0.208863
Sum of Mulliken atomic charges =   0.00000
Mulliken charges with hydrogens summed into heavy atoms:
             1
    1  C    0.638838
    2  O   -0.515302
    3  N   -0.123537
Sum of Mulliken charges with hydrogens summed into heavy atoms =   0.00000
Electronic spatial extent (au):  =            153.6971
Charge=              0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=              2.8315    Y=              2.6568    Z=              1.7089  Tot=              4.2422
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=            -19.1240   YY=            -15.2644   ZZ=            -18.0567
  XY=             -0.7969   XZ=              1.7988   YZ=             -1.4714
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=             -1.6423   YY=              2.2173   ZZ=             -0.5750
  XY=             -0.7969   XZ=              1.7988   YZ=             -1.4714
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=              8.7791  YYY=              1.9268  ZZZ=              1.7204  XYY=              0.6067
 XXY=              2.2689  XXZ=              2.4110  XZZ=             -0.9894  YZZ=             -0.4217
 YYZ=              1.9035  XYZ=             -2.0505
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=           -117.0069 YYYY=            -36.0086 ZZZZ=            -17.7943 XXXY=              3.9806
XXXZ=              3.6712 YYYX=             -1.3785 YYYZ=             -1.4209 ZZZX=              2.3318
ZZZY=             -1.6129 XXYY=            -24.9712 XXZZ=            -24.1946 YYZZ=             -9.2652
XXYZ=             -2.6141 YYXZ=              1.6979 ZZXY=             -0.2055
N-N= 6.759905342259D+01 E-N=-5.323220748779D+02  KE= 1.678106427240D+02
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
     1        6           0.104388877    0.005354930    0.148329228
     2        8          -0.033266758    0.003005438   -0.136997208
     3        7          -0.059987370    0.036499408   -0.047127446
     4        1           0.005959237    0.005070581    0.050548695
     5        1          -0.027373473   -0.045243762   -0.014788304
     6        1           0.010279486   -0.004686595    0.000035036
-------------------------------------------------------------------
Cartesian Forces:  Max     0.148329228 RMS     0.060425312

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.136997208 RMS     0.048286250
Search for a local minimum.
Step number   1 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Second derivative matrix not updated -- first step.
The second derivative matrix:
                       R1        R2        R3        R4        R5
          R1           0.74643
          R2           0.00000   0.30367
          R3           0.00000   0.00000   0.34813
          R4           0.00000   0.00000   0.00000   0.37230
          R5           0.00000   0.00000   0.00000   0.00000   0.37230
          A1           0.00000   0.00000   0.00000   0.00000   0.00000
          A2           0.00000   0.00000   0.00000   0.00000   0.00000
          A3           0.00000   0.00000   0.00000   0.00000   0.00000
          A4           0.00000   0.00000   0.00000   0.00000   0.00000
          A5           0.00000   0.00000   0.00000   0.00000   0.00000
          A6           0.00000   0.00000   0.00000   0.00000   0.00000
          D1           0.00000   0.00000   0.00000   0.00000   0.00000
          D2           0.00000   0.00000   0.00000   0.00000   0.00000
          D3           0.00000   0.00000   0.00000   0.00000   0.00000
          D4           0.00000   0.00000   0.00000   0.00000   0.00000
                         A1        A2        A3        A4        A5
          A1           0.14667
          A2          -0.07333   0.11667
          A3          -0.07333  -0.04333   0.11667
          A4           0.00000   0.00000   0.00000   0.13594
          A5           0.00000   0.00000   0.00000  -0.02406   0.13594
          A6           0.00000   0.00000   0.00000  -0.04812  -0.04812
          D1           0.00000   0.00000   0.00000  -0.00479  -0.00479
          D2           0.00000   0.00000   0.00000   0.00479   0.00479
          D3           0.00000   0.00000   0.00000  -0.00479  -0.00479
          D4           0.00000   0.00000   0.00000   0.00479   0.00479
                         A6        D1        D2        D3        D4
          A6           0.06376
          D1          -0.00958   0.00995
```

```
          D2           0.00958  -0.00765   0.00995
          D3          -0.00958   0.00880  -0.00880   0.00995
          D4           0.00958  -0.00880   0.00880  -0.00765   0.00995
    Eigenvalues ---    0.00230   0.00230   0.05082   0.16000   0.16000
    Eigenvalues ---    0.16000   0.22000   0.30367   0.34813   0.37230
    Eigenvalues ---    0.37230   0.746431000.000001000.000001000.00000
RFO step:  Lambda=-6.90357543D-02 EMin= 2.30000000D-03
Linear search not attempted -- first point.
Maximum step size (   0.300) exceeded in Quadratic search.
   -- Step size scaled by   0.727
Iteration  1 RMS(Cart)=  0.08313370 RMS(Int)=  0.00396200
Iteration  2 RMS(Cart)=  0.00495126 RMS(Int)=  0.00006952
Iteration  3 RMS(Cart)=  0.00001249 RMS(Int)=  0.00006833
Iteration  4 RMS(Cart)=  0.00000000 RMS(Int)=  0.00006833
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.40940  -0.13700   0.00000  -0.12218  -0.12218   2.28722
   R2        2.87238  -0.07296   0.00000  -0.14236  -0.14236   2.73002
   R3        2.05980  -0.00841   0.00000  -0.01467  -0.01467   2.04513
   R4        2.02201  -0.05055   0.00000  -0.08330  -0.08330   1.93871
   R5        2.02201  -0.05477   0.00000  -0.09026  -0.09026   1.93175
   A1        1.91063   0.05749   0.00000   0.14465   0.14465   2.05528
   A2        2.18628  -0.02266   0.00000  -0.05301  -0.05302   2.13326
   A3        2.18628  -0.03483   0.00000  -0.09164  -0.09165   2.09463
   A4        1.91063   0.01087   0.00000   0.03422   0.03430   1.94494
   A5        1.91063  -0.00680   0.00000  -0.02189  -0.02180   1.88884
   A6        1.91063  -0.00236   0.00000  -0.00809  -0.00791   1.90272
   D1        3.14159   0.00361   0.00000   0.03598   0.03605  -3.10554
   D2       -1.04720   0.00322   0.00000   0.03362   0.03355  -1.01365
   D3        0.00000   0.00414   0.00000   0.04136   0.04143   0.04143
   D4        2.09440   0.00375   0.00000   0.03900   0.03893   2.13332
         Item               Value     Threshold  Converged?
Maximum Force            0.136997     0.000450     NO
RMS     Force            0.048286     0.000300     NO
Maximum Displacement     0.187231     0.001800     NO
RMS     Displacement     0.082824     0.001200     NO
Predicted change in Energy=-3.505671D-02
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.067717    0.005170    0.033790
     2          8           0       -0.043450    0.013600    1.238991
     3          7           0        1.402518    0.001928   -0.518798
     4          1           0        1.383894    0.029123   -1.544190
     5          1           0        1.893855    0.828753   -0.172510
     6          1           0       -0.790903   -0.004924   -0.624928
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.210346   0.000000
    3  N    1.444665   2.276133   0.000000
    4  H    2.054974   3.127882   1.025921   0.000000
    5  H    2.013859   2.531790   1.022236   1.667625   0.000000
    6  H    1.082238   2.008289   2.195997   2.361343   2.847388
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.190738    0.428177    0.032741
     2          8           0       -1.171096   -0.279288   -0.024971
     3          7           0        1.102013   -0.200306   -0.111690
     4          1           0        1.863045    0.480649   -0.013484
     5          1           0        1.195032   -0.911210    0.616959
     6          1           0       -0.258973    1.497944    0.181681
---------------------------------------------------------------------
Rotational constants (GHZ):     63.9854308     11.2783517      9.8031375
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        70.2274379142 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
```

```
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.911973933     A.U. after   14 cycles
           Convg  =    0.1930D-08             -V/T =  2.0036
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
     1        6           0.048867526   -0.001984686    0.056319488
     2        8          -0.009322433    0.004285262   -0.048046046
     3        7          -0.041099708    0.022065470   -0.021244455
     4        1           0.002698643    0.001167043    0.021018208
     5        1          -0.003063629   -0.020433549   -0.001852013
     6        1           0.001919601   -0.005099540   -0.006195183
-------------------------------------------------------------------
Cartesian Forces:  Max     0.056319488 RMS     0.025335281

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.046955704 RMS     0.019361763
Search for a local minimum.
Step number   2 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points    1    2
DE= -3.64D-02 DEPred=-3.51D-02 R= 1.04D+00
SS=  1.41D+00  RLast= 3.00D-01 DXNew= 5.0454D-01 9.0000D-01
Trust test= 1.04D+00 RLast= 3.00D-01 DXMaxT set to 5.05D-01
The second derivative matrix:
                       R1        R2        R3        R4        R5
          R1           0.74775
          R2          -0.02158   0.28470
          R3           0.01743   0.00562   0.35117
          R4          -0.00291  -0.00866   0.00553   0.37021
          R5           0.00958  -0.00437   0.00751   0.00191   0.37948
          A1          -0.00358   0.00630  -0.00645  -0.00001  -0.00460
          A2           0.01164   0.00148   0.00381   0.00335   0.00595
          A3          -0.00806  -0.00778   0.00264  -0.00334  -0.00135
          A4          -0.00390  -0.00019  -0.00151  -0.00107  -0.00211
          A5           0.03288   0.01211   0.00456   0.01066   0.01354
          A6           0.00189   0.00047   0.00044   0.00058   0.00087
          D1          -0.00613  -0.00238  -0.00076  -0.00201  -0.00248
          D2           0.01449   0.00571   0.00172   0.00475   0.00581
          D3          -0.00851  -0.00331  -0.00104  -0.00278  -0.00343
          D4           0.01211   0.00477   0.00143   0.00397   0.00486
                       A1        A2        A3        A4        A5
          A1           0.14904
          A2          -0.07796   0.12039
          A3          -0.07108  -0.04243   0.11350
          A4           0.00159  -0.00140  -0.00019   0.13646
          A5          -0.01196   0.00642   0.00555  -0.02666   0.14232
          A6          -0.00072   0.00049   0.00023  -0.04831  -0.04741
          D1           0.00221  -0.00113  -0.00108  -0.00432  -0.00580
          D2          -0.00522   0.00264   0.00258   0.00371   0.00705
          D3           0.00307  -0.00157  -0.00150  -0.00415  -0.00618
          D4          -0.00436   0.00220   0.00216   0.00389   0.00667
                       A6        D1        D2        D3        D4
          A6           0.06382
          D1          -0.00970   0.01010
          D2           0.00986  -0.00799   0.01070
          D3          -0.00974   0.00901  -0.00927   0.01024
```

```
          D4           0.00981  -0.00908   0.00942  -0.00804   0.01047
Use linear search instead of GDIIS.
    Eigenvalues ---    0.00228   0.00230   0.05052   0.15562   0.16000
    Eigenvalues ---    0.16170   0.22627   0.28500   0.34904   0.37098
    Eigenvalues ---    0.38395   0.752671000.000001000.000001000.00000
RFO step:  Lambda=-8.35255982D-03 EMin= 2.27567321D-03
Quartic linear search produced a step of  0.54222.
Maximum step size (   0.505) exceeded in Quadratic search.
   -- Step size scaled by   0.813
Iteration  1 RMS(Cart)=  0.10211119 RMS(Int)=  0.04076054
Iteration  2 RMS(Cart)=  0.03118619 RMS(Int)=  0.00267976
Iteration  3 RMS(Cart)=  0.00117366 RMS(Int)=  0.00241892
Iteration  4 RMS(Cart)=  0.00000106 RMS(Int)=  0.00241892
Iteration  5 RMS(Cart)=  0.00000001 RMS(Int)=  0.00241892
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.28722  -0.04696  -0.06625  -0.00523  -0.07148   2.21574
   R2        2.73002  -0.03752  -0.07719  -0.04381  -0.12101   2.60902
   R3        2.04513   0.00230  -0.00795   0.01839   0.01043   2.05557
   R4        1.93871  -0.02103  -0.04517  -0.01074  -0.05590   1.88281
   R5        1.93175  -0.01863  -0.04894   0.00192  -0.04703   1.88472
   A1        2.05528   0.02505   0.07843   0.01544   0.09312   2.14841
   A2        2.13326  -0.00626  -0.02875   0.02007  -0.00943   2.12383
   A3        2.09463  -0.01879  -0.04969  -0.03514  -0.08558   2.00905
   A4        1.94494   0.00415   0.01860   0.02165   0.03641   1.98135
   A5        1.88884   0.00731  -0.01182   0.09888   0.08320   1.97204
   A6        1.90272  -0.00060  -0.00429   0.05120   0.04080   1.94352
   D1       -3.10554   0.00147   0.01955   0.19746   0.21480  -2.89073
   D2       -1.01365   0.00793   0.01819   0.33714   0.35749  -0.65616
   D3        0.04143   0.00121   0.02246   0.12382   0.14412   0.18555
   D4        2.13332   0.00767   0.02111   0.26349   0.28680   2.42012
       Item               Value     Threshold  Converged?
Maximum Force            0.046956     0.000450     NO
RMS     Force            0.019362     0.000300     NO
Maximum Displacement     0.223045     0.001800     NO
RMS     Displacement     0.128623     0.001200     NO
Predicted change in Energy=-1.441809D-02
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.101485   -0.011468    0.051094
     2          8           0       -0.062191    0.117038    1.205000
     3          7           0        1.346774    0.033881   -0.543335
     4          1           0        1.311148    0.136234   -1.533762
     5          1           0        1.951397    0.710723   -0.129782
     6          1           0       -0.734982   -0.112756   -0.636861
---------------------------------------------------------------------
                   Distance matrix (angstroms):
                   1          2          3          4          5
    1  C    0.000000
    2  O    1.172520   0.000000
    3  N    1.380632   2.246947   0.000000
    4  H    1.999217   3.063861   0.996339   0.000000
    5  H    1.994103   2.487697   0.997352   1.646546   0.000000
    6  H    1.087759   1.974311   2.089009   2.247905   2.855150
                   6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.178155    0.385914    0.001521
     2          8           0       -1.161269   -0.253043   -0.003371
     3          7           0        1.082187   -0.169163   -0.096320
     4          1           0        1.814356    0.461366    0.146686
     5          1           0        1.167226   -1.031872    0.396845
     6          1           0       -0.197802    1.463510    0.148557
---------------------------------------------------------------------
Rotational constants (GHZ):     72.8138288     11.6873095     10.1956966
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.2240072189 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
```

```
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.924440010     A.U. after   14 cycles
           Convg  =    0.3922D-08             -V/T =  2.0015
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
     1        6           0.012852882    0.008554944   -0.023091553
     2        8          -0.007839871    0.002151162    0.033123723
     3        7          -0.013042601    0.004679129   -0.009606801
     4        1           0.002211767   -0.000750654   -0.002771440
     5        1           0.005229809   -0.005346600    0.006160836
     6        1           0.000588014   -0.009287981   -0.003814765
-------------------------------------------------------------------
Cartesian Forces:  Max     0.033123723 RMS     0.011612646

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.033928040 RMS     0.010078924
Search for a local minimum.
Step number   3 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points    2    3
DE= -1.25D-02 DEPred=-1.44D-02 R= 8.65D-01
SS=  1.41D+00  RLast= 5.73D-01 DXNew= 8.4853D-01 1.7186D+00
Trust test= 8.65D-01 RLast= 5.73D-01 DXMaxT set to 8.49D-01
The second derivative matrix:
                      R1        R2        R3        R4        R5
          R1          0.98859
          R2          0.04944   0.29356
          R3          0.02457   0.00974   0.35105
          R4          0.05265   0.00239   0.00806   0.38068
          R5          0.05641   0.00407   0.00979   0.01034   0.38620
          A1          -0.02752  0.00964  -0.00889  -0.00095  -0.00463
          A2          0.02588   0.00398   0.00452   0.00589   0.00796
          A3          0.00435  -0.01245   0.00439  -0.00415  -0.00264
          A4          0.00855   0.00706  -0.00174   0.00338   0.00190
          A5          0.02768   0.01352   0.00392   0.01075   0.01384
          A6          0.00750   0.00242   0.00056   0.00200   0.00210
          D1          -0.04522  -0.02076  -0.00078  -0.01405  -0.01312
          D2          -0.00347  -0.00079   0.00139   0.00008   0.00179
          D3          0.00080   -0.00049  -0.00078  -0.00060  -0.00159
          D4          0.04255   0.01948   0.00139   0.01352   0.01332
                      A1        A2        A3        A4        A5
          A1          0.14248
          A2          -0.07792  0.12100
          A3          -0.06515  -0.04286  0.10840
          A4          -0.00273  -0.00017  0.00292   0.13604
          A5          -0.01398  0.00652   0.00730  -0.02780   0.14172
          A6          -0.00154  0.00086   0.00073  -0.04811  -0.04760
          D1          0.01200   -0.00440  -0.00782  -0.00431  -0.00329
          D2          -0.00240  0.00141   0.00083   0.00314   0.00773
          D3          0.00208   -0.00101  -0.00097  -0.00369  -0.00639
          D4          -0.01231  0.00480   0.00767   0.00376   0.00462
                      A6        D1        D2        D3        D4
          A6          0.06394
          D1          -0.01044  0.01256
          D2          0.00947   -0.00576  0.01192
          D3          -0.00953  0.00754   -0.00995  0.01060
```

```
          D4           0.01038  -0.01077   0.00772  -0.00690   0.01160
Use linear search instead of GDIIS.
    Eigenvalues ---    0.00181   0.00347   0.04430   0.15090   0.15914
    Eigenvalues ---    0.16466   0.21788   0.29446   0.34904   0.37270
    Eigenvalues ---    0.38902   1.010851000.000001000.000001000.00000
RFO step:  Lambda=-1.26548631D-02 EMin= 1.81234600D-03
Quartic linear search produced a step of  0.16904.
Iteration  1 RMS(Cart)=  0.07582575 RMS(Int)=  0.14184519
Iteration  2 RMS(Cart)=  0.06168309 RMS(Int)=  0.07020752
Iteration  3 RMS(Cart)=  0.05436251 RMS(Int)=  0.02700336
Iteration  4 RMS(Cart)=  0.00338810 RMS(Int)=  0.02670614
Iteration  5 RMS(Cart)=  0.00013455 RMS(Int)=  0.02670572
Iteration  6 RMS(Cart)=  0.00000908 RMS(Int)=  0.02670572
Iteration  7 RMS(Cart)=  0.00000064 RMS(Int)=  0.02670572
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.21574   0.03393  -0.01208   0.01606   0.00398   2.21972
   R2        2.60902  -0.00242  -0.02045  -0.05045  -0.07091   2.53811
   R3        2.05557   0.00283   0.00176   0.00936   0.01113   2.06669
   R4        1.88281   0.00260  -0.00945  -0.01454  -0.02399   1.85882
   R5        1.88472   0.00210  -0.00795  -0.01412  -0.02206   1.86266
   A1        2.14841   0.00733   0.01574   0.07914   0.04301   2.19141
   A2        2.12383   0.00009  -0.00159   0.01053  -0.05383   2.07001
   A3        2.00905  -0.00687  -0.01447  -0.05159  -0.12104   1.88801
   A4        1.98135   0.00500   0.00616   0.05619   0.05521   2.03656
   A5        1.97204   0.00282   0.01406   0.04985   0.05676   2.02880
   A6        1.94352   0.00100   0.00690   0.04488   0.04241   1.98593
   D1       -2.89073  -0.00528   0.03631  -0.19088  -0.14291  -3.03364
   D2       -0.65616   0.00302   0.06043  -0.03453   0.04298  -0.61319
   D3        0.18555   0.00426   0.02436   0.46219   0.46947   0.65502
   D4        2.42012   0.01256   0.04848   0.61854   0.65536   3.07548
         Item               Value     Threshold  Converged?
Maximum Force            0.033928     0.000450     NO
RMS     Force            0.010079     0.000300     NO
Maximum Displacement     0.359602     0.001800     NO
RMS     Displacement     0.175515     0.001200     NO
Predicted change in Energy=-1.103621D-02
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.082070    0.164890    0.041263
     2          8           0       -0.094343    0.138152    1.202257
     3          7           0        1.276905    0.101400   -0.568884
     4          1           0        1.282204    0.228894   -1.544216
     5          1           0        2.026617    0.543365   -0.106113
     6          1           0       -0.659822   -0.303050   -0.611954
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.174625   0.000000
    3  N    1.343109   2.240226   0.000000
    4  H    1.989513   3.073472   0.983644   0.000000
    5  H    1.986510   2.524777   0.985676   1.649601   0.000000
    6  H    1.093647   1.950843   1.978977   2.218905   2.861686
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.163015    0.357031    0.103594
     2          8           0       -1.171118   -0.232140   -0.024268
     3          7           0        1.066765   -0.149188   -0.084362
     4          1           0        1.824528    0.432859    0.149242
     5          1           0        1.194528   -1.091482    0.175090
     6          1           0       -0.139373    1.417871   -0.161214
---------------------------------------------------------------------
Rotational constants (GHZ):     78.8994282     11.7174788     10.3226302
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.8617078693 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
```

```
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on              energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.913338537     A.U. after   14 cycles
           Convg  =    0.4614D-08             -V/T =  2.0007
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
     1        6          -0.009409869   -0.084478740   -0.020688454
     2        8          -0.005007832    0.032611424    0.040629467
     3        7           0.013536410    0.023297288   -0.005290059
     4        1           0.000887761    0.001174952   -0.013922677
     5        1           0.013329152    0.002772093    0.007788360
     6        1          -0.013335622    0.024622983   -0.008516636
-------------------------------------------------------------------
Cartesian Forces:  Max     0.084478740 RMS     0.026294504

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.040167745 RMS     0.020817179
Search for a local minimum.
Step number   4 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points    2    4    3
DE=  1.11D-02 DEPred=-1.10D-02 R=-1.01D+00
Trust test=-1.01D+00 RLast= 8.40D-01 DXMaxT set to 4.24D-01
The second derivative matrix:
                       R1        R2        R3        R4        R5
          R1           0.72345
          R2           0.07183   0.31163
          R3           0.00299   0.01173   0.34929
          R4           0.03428   0.01086   0.00662   0.38180
          R5           0.04241   0.01323   0.00871   0.01214   0.38866
          A1          -0.09020   0.01293  -0.01401  -0.00598  -0.00874
          A2           0.03757   0.00515   0.00549   0.00744   0.00944
          A3           0.05905   0.00095   0.00900   0.00588   0.00746
          A4          -0.02769   0.00718  -0.00471  -0.00015  -0.00119
          A5           0.01011   0.01469   0.00248   0.00943   0.01279
          A6          -0.00224   0.00209  -0.00024   0.00093   0.00112
          D1          -0.01769  -0.00197   0.00164  -0.00482  -0.00322
          D2          -0.02044   0.01851   0.00015   0.00510   0.00804
          D3           0.01063  -0.02202  -0.00015  -0.00710  -0.00934
          D4           0.00788  -0.00153  -0.00164   0.00282   0.00192
                       A1        A2        A3        A4        A5
          A1           0.12786
          A2          -0.07538   0.12071
          A3          -0.05402  -0.04333   0.11337
          A4          -0.01100   0.00111   0.00774   0.13152
          A5          -0.01810   0.00726   0.01065  -0.03015   0.14056
          A6          -0.00373   0.00117   0.00170  -0.04927  -0.04823
          D1           0.01639  -0.00334   0.00555  -0.00366  -0.00179
          D2          -0.00820   0.00408   0.02045  -0.00182   0.00633
          D3           0.00647  -0.00367  -0.02167   0.00071  -0.00543
          D4          -0.01811   0.00375  -0.00677   0.00255   0.00269
                       A6        D1        D2        D3        D4
          A6           0.06365
          D1          -0.01064   0.03202
          D2           0.00782   0.01490   0.02683
          D3          -0.00798  -0.01536  -0.02784   0.03168
          D4           0.01048  -0.03248  -0.01591   0.01919   0.03576
```

```
Use linear search instead of GDIIS.
    Eigenvalues ---    0.00224   0.02387   0.08982   0.14256   0.16313
    Eigenvalues ---    0.16594   0.18981   0.30671   0.34906   0.37262
    Eigenvalues ---    0.39450   0.768971000.000001000.000001000.00000
RFO step:  Lambda=-1.20636060D-02 EMin= 2.24270042D-03
Quartic linear search produced a step of -0.72038.
Maximum step size (   0.424) exceeded in Quadratic search.
   -- Step size scaled by   0.601
Iteration  1 RMS(Cart)=  0.07529349 RMS(Int)=  0.03989699
Iteration  2 RMS(Cart)=  0.02441570 RMS(Int)=  0.00334946
Iteration  3 RMS(Cart)=  0.00106741 RMS(Int)=  0.00317612
Iteration  4 RMS(Cart)=  0.00000097 RMS(Int)=  0.00317612
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   R1        2.21972   0.04017  -0.00287   0.05554   0.05267   2.27239
   R2        2.53811   0.02859   0.05108  -0.02103   0.03005   2.56816
   R3        2.06669   0.00360  -0.00802   0.01041   0.00239   2.06909
   R4        1.85882   0.01396   0.01728   0.00212   0.01940   1.87822
   R5        1.86266   0.01504   0.01589  -0.00063   0.01526   1.87792
   A1        2.19141   0.00565  -0.03098   0.08771   0.05176   2.24317
   A2        2.07001   0.00322   0.03877   0.00378   0.03758   2.10759
   A3        1.88801   0.02030   0.08720  -0.03787   0.04436   1.93236
   A4        2.03656   0.00120  -0.03977   0.05953   0.02408   2.06064
   A5        2.02880   0.00275  -0.04089   0.03143  -0.00509   2.02371
   A6        1.98593  -0.00058  -0.03055   0.03332   0.00827   1.99421
   D1       -3.03364   0.02742   0.10295   0.13225   0.23673  -2.79691
   D2       -0.61319   0.03164  -0.03096   0.30991   0.27747  -0.33572
   D3        0.65502  -0.02865  -0.33820   0.03817  -0.29854   0.35648
   D4        3.07548  -0.02443  -0.47211   0.21583  -0.25781   2.81767
         Item               Value     Threshold  Converged?
Maximum Force            0.040168     0.000450     NO
RMS     Force            0.020817     0.000300     NO
Maximum Displacement     0.275645     0.001800     NO
RMS     Displacement     0.092246     0.001200     NO
Predicted change in Energy=-8.354170D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.109596    0.019025    0.065826
     2          8           0       -0.119399    0.182186    1.234988
     3          7           0        1.302222    0.093149   -0.581519
     4          1           0        1.292245    0.228493   -1.566122
     5          1           0        2.023646    0.586747   -0.108814
     6          1           0       -0.694680   -0.235949   -0.632005
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.202498   0.000000
    3  N    1.359009   2.308383   0.000000
    4  H    2.026274   3.137052   0.993912   0.000000
    5  H    2.004094   2.561662   0.993751   1.669443   0.000000
    6  H    1.094915   1.997860   2.024468   2.244137   2.887880
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.159009    0.358201   -0.002373
     2          8           0       -1.206713   -0.231876    0.008853
     3          7           0        1.098910   -0.151614   -0.070467
     4          1           0        1.853389    0.423971    0.225038
     5          1           0        1.194125   -1.109066    0.178050
     6          1           0       -0.132123    1.452194    0.033601
---------------------------------------------------------------------
Rotational constants (GHZ):     79.1539319     11.1320452      9.8129243
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        71.5071569285 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
```

```
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.928639941     A.U. after   14 cycles
            Convg  =    0.6748D-08             -V/T =  2.0023
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
     1        6          -0.020365169   -0.000422043    0.006597723
     2        8           0.015912002   -0.001589719   -0.022185310
     3        7           0.000279222    0.006810727    0.010853363
     4        1          -0.002276152   -0.001872569   -0.001849115
     5        1           0.005703516   -0.001264729    0.003707365
     6        1           0.000746581   -0.001661667    0.002875974
-------------------------------------------------------------------
Cartesian Forces:  Max     0.022185310 RMS     0.008951056

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.024816160 RMS     0.009048985
Search for a local minimum.
Step number   5 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points    4    3    5
DE= -4.20D-03 DEPred=-8.35D-03 R= 5.03D-01
SS=  1.41D+00  RLast= 5.75D-01 DXNew= 7.1352D-01 1.7248D+00
Trust test= 5.03D-01 RLast= 5.75D-01 DXMaxT set to 7.14D-01
The second derivative matrix:
                       R1        R2        R3        R4        R5
          R1           0.92300
          R2           0.09653   0.31481
          R3           0.01981   0.01381   0.35071
          R4           0.03020   0.01029   0.00632   0.37919
          R5           0.01377   0.00955   0.00637   0.00806   0.38470
          A1           0.05729   0.03160  -0.00173   0.00139  -0.01196
          A2           0.00039   0.00046   0.00239   0.00576   0.01055
          A3          -0.00249  -0.00672   0.00387   0.00318   0.00942
          A4          -0.00334   0.01019  -0.00267  -0.00035  -0.00416
          A5          -0.00928   0.01217   0.00089   0.00691   0.01054
          A6          -0.01103   0.00097  -0.00097   0.00037   0.00110
          D1           0.02117   0.00312   0.00487  -0.00196  -0.00251
          D2           0.01349   0.02287   0.00300   0.00567   0.00533
          D3           0.00492  -0.02281  -0.00065  -0.00596  -0.00674
          D4          -0.00276  -0.00305  -0.00252   0.00166   0.00110
                       A1        A2        A3        A4        A5
          A1           0.19701
          A2          -0.09347   0.12543
          A3          -0.08416  -0.03546   0.12654
          A4           0.00581  -0.00314   0.00067   0.13446
          A5          -0.02125   0.00824   0.01233  -0.03218   0.13931
          A6          -0.00736   0.00213   0.00331  -0.05026  -0.04818
          D1           0.03124  -0.00730  -0.00097   0.00064  -0.00168
          D2           0.01217  -0.00112   0.01190   0.00217   0.00435
          D3          -0.00180  -0.00167  -0.01846  -0.00009  -0.00373
          D4          -0.02088   0.00452  -0.00558   0.00143   0.00230
                       A6        D1        D2        D3        D4
          A6           0.06383
          D1          -0.01136   0.03491
          D2           0.00666   0.01999   0.03214
          D3          -0.00743  -0.01803  -0.02941   0.03156
          D4           0.01059  -0.03294  -0.01726   0.02017   0.03586
Use linear search instead of GDIIS.
```

```
    Eigenvalues ---    0.00362   0.02995   0.09377   0.14997   0.16319
    Eigenvalues ---    0.16718   0.26883   0.31554   0.35017   0.37340
    Eigenvalues ---    0.39644   0.945971000.000001000.000001000.00000
RFO step:  Lambda=-3.60831782D-03 EMin= 3.61979581D-03
Quartic linear search produced a step of -0.15050.
Iteration  1 RMS(Cart)=  0.09890977 RMS(Int)=  0.01053257
Iteration  2 RMS(Cart)=  0.00873824 RMS(Int)=  0.00072897
Iteration  3 RMS(Cart)=  0.00007284 RMS(Int)=  0.00072518
Iteration  4 RMS(Cart)=  0.00000001 RMS(Int)=  0.00072518
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   R1        2.27239  -0.02482  -0.00853  -0.02272  -0.03124   2.24115
   R2        2.56816  -0.00260   0.00615   0.00273   0.00888   2.57704
   R3        2.06909  -0.00199  -0.00204  -0.00634  -0.00838   2.06071
   R4        1.87822   0.00160   0.00069   0.00500   0.00569   1.88391
   R5        1.87792   0.00528   0.00102   0.01020   0.01122   1.88914
   A1        2.24317  -0.01853  -0.01426  -0.06013  -0.07427   2.16891
   A2        2.10759   0.00758   0.00244   0.01758   0.02016   2.12775
   A3        1.93236   0.01092   0.01154   0.04240   0.05407   1.98643
   A4        2.06064  -0.00270  -0.01193  -0.00233  -0.01287   2.04777
   A5        2.02371   0.00331  -0.00778   0.01265   0.00627   2.02998
   A6        1.99421   0.00191  -0.00763   0.02116   0.01528   2.00949
   D1       -2.79691  -0.00249  -0.01412   0.21562   0.20197  -2.59494
   D2       -0.33572   0.00193  -0.04823   0.26926   0.22056  -0.11515
   D3        0.35648  -0.00001  -0.02572   0.23075   0.20550   0.56197
   D4        2.81767   0.00441  -0.05983   0.28439   0.22409   3.04176
        Item               Value     Threshold  Converged?
Maximum Force            0.024816     0.000450     NO
RMS     Force            0.009049     0.000300     NO
Maximum Displacement     0.199410     0.001800     NO
RMS     Displacement     0.104395     0.001200     NO
Predicted change in Energy=-2.345716D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.090026    0.011398    0.041304
     2          8           0       -0.083602    0.268475    1.185978
     3          7           0        1.295041    0.098872   -0.591141
     4          1           0        1.287479    0.334016   -1.559907
     5          1           0        2.044588    0.497506   -0.063267
     6          1           0       -0.719902   -0.336616   -0.600611
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.185965   0.000000
    3  N    1.363709   2.255565   0.000000
    4  H    2.025303   3.069860   0.996924   0.000000
    5  H    2.016817   2.478358   0.999690   1.685194   0.000000
    6  H    1.090481   1.990706   2.061488   2.323698   2.937159
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.171398    0.387497   -0.018597
     2          8           0       -1.167082   -0.255291    0.025571
     3          7           0        1.083872   -0.143369   -0.065274
     4          1           0        1.817683    0.378442    0.362620
     5          1           0        1.149790   -1.135120    0.041798
     6          1           0       -0.189531    1.477608   -0.040491
---------------------------------------------------------------------
Rotational constants (GHZ):     72.8282262     11.6589012     10.1284793
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.0607392190 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
```

```
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
 Harris functional with IExCor=  205 diagonalized for initial guess.
 ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
 HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 ints in memory in canonical form, NReq=1726457.
 SCF Done:  E(RHF) =  -168.929105243     A.U. after   13 cycles
            Convg  =    0.4944D-08             -V/T =  2.0019
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.003769413    0.004206586   -0.005358657
      2        8          -0.002153565   -0.002352164    0.011109024
      3        7          -0.001755052    0.000665940   -0.003176722
      4        1           0.001584063   -0.004241165   -0.000497256
      5        1          -0.003176445    0.001055759   -0.000000142
      6        1           0.001731585    0.000665045   -0.002076247
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.011109024 RMS     0.003708212

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.010527660 RMS     0.003862925
 Search for a local minimum.
 Step number   6 out of a maximum of   25
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    5    6
 DE= -4.65D-04 DEPred=-2.35D-03 R= 1.98D-01
 Trust test= 1.98D-01 RLast= 4.39D-01 DXMaxT set to 7.14D-01
 The second derivative matrix:
                        R1        R2        R3        R4        R5
          R1           0.91106
          R2           0.08245   0.31289
          R3           0.01332   0.01250   0.34992
          R4           0.03164   0.01121   0.00677   0.37906
          R5           0.01757   0.01257   0.00780   0.00768   0.38364
          A1           0.02488   0.01997  -0.00786   0.00390  -0.00428
          A2           0.01735   0.00476   0.00482   0.00454   0.00671
          A3          -0.00505  -0.00128   0.00613   0.00304   0.00940
          A4           0.01384   0.00961  -0.00233  -0.00132  -0.00756
          A5          -0.01363   0.01417   0.00161   0.00706   0.01121
          A6           0.00149   0.00277   0.00023  -0.00046  -0.00160
          D1          -0.01515   0.00021   0.00237   0.00032   0.00510
          D2          -0.00635   0.02270   0.00224   0.00684   0.00934
          D3          -0.00787  -0.02358  -0.00142  -0.00517  -0.00409
          D4           0.00094  -0.00109  -0.00154   0.00134   0.00016
                         A1        A2        A3        A4        A5
          A1           0.15716
          A2          -0.07585   0.11812
          A3          -0.07580  -0.04087   0.13086
          A4           0.01473  -0.00528  -0.00763   0.13929
          A5          -0.02015   0.00680   0.01550  -0.03604   0.14118
          A6           0.00314  -0.00179  -0.00147  -0.04988  -0.04991
          D1           0.00491   0.00163   0.01422  -0.00372   0.00447
          D2           0.00034   0.00225   0.02102  -0.00221   0.00839
          D3          -0.01061   0.00120  -0.01296  -0.00199  -0.00144
          D4          -0.01518   0.00183  -0.00617  -0.00049   0.00248
                         A6        D1        D2        D3        D4
          A6           0.06216
          D1          -0.00853   0.03293
          D2           0.00696   0.02274   0.03588
          D3          -0.00666  -0.01803  -0.02804   0.03180
          D4           0.00883  -0.02822  -0.01491   0.02180   0.03510
 Use linear search instead of GDIIS.
     Eigenvalues ---    0.00982   0.02810   0.09296   0.14868   0.16126
     Eigenvalues ---    0.17150   0.24344   0.30620   0.34886   0.37315
     Eigenvalues ---    0.39537   0.926941000.000001000.000001000.00000
 RFO step:  Lambda=-1.24539332D-03 EMin= 9.82495460D-03
```

```
Quartic linear search produced a step of -0.43277.
Iteration  1 RMS(Cart)=  0.08079565 RMS(Int)=  0.02240543
Iteration  2 RMS(Cart)=  0.01784523 RMS(Int)=  0.00101299
Iteration  3 RMS(Cart)=  0.00038759 RMS(Int)=  0.00092178
Iteration  4 RMS(Cart)=  0.00000015 RMS(Int)=  0.00092178
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   R1        2.24115   0.01053   0.01352  -0.00882   0.00470   2.24585
   R2        2.57704  -0.00142  -0.00384  -0.01115  -0.01499   2.56204
   R3        2.06071  -0.00028   0.00363  -0.00258   0.00105   2.06176
   R4        1.88391  -0.00053  -0.00246   0.00118  -0.00128   1.88263
   R5        1.88914  -0.00196  -0.00486   0.00538   0.00053   1.88967
   A1        2.16891   0.00411   0.03214  -0.03107   0.00100   2.16990
   A2        2.12775   0.00065  -0.00872   0.01908   0.01028   2.13803
   A3        1.98643  -0.00481  -0.02340   0.01165  -0.01182   1.97461
   A4        2.04777   0.00387   0.00557   0.02290   0.02661   2.07439
   A5        2.02998  -0.00346  -0.00271   0.01727   0.01269   2.04267
   A6        2.00949   0.00060  -0.00661   0.03100   0.02221   2.03170
   D1       -2.59494  -0.00502  -0.08741  -0.18530  -0.27320  -2.86814
   D2       -0.11515  -0.00334  -0.09545  -0.06884  -0.16379  -0.27895
   D3        0.56197  -0.00160  -0.08893  -0.16115  -0.25058   0.31139
   D4        3.04176   0.00008  -0.09698  -0.04469  -0.14117   2.90059
         Item               Value     Threshold  Converged?
Maximum Force            0.010528     0.000450     NO
RMS     Force            0.003863     0.000300     NO
Maximum Displacement     0.221353     0.001800     NO
RMS     Displacement     0.096134     0.001200     NO
Predicted change in Energy=-1.336804D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.089484    0.025089    0.047654
     2          8           0       -0.072301    0.179942    1.214815
     3          7           0        1.287878    0.126631   -0.578179
     4          1           0        1.306089    0.216881   -1.570163
     5          1           0        2.025613    0.578692   -0.076855
     6          1           0       -0.723133   -0.253583   -0.624918
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.188453   0.000000
    3  N    1.355775   2.251168   0.000000
    4  H    2.033284   3.107640   0.996247   0.000000
    5  H    2.017567   2.495728   0.999969   1.696641   0.000000
    6  H    1.091035   1.999036   2.047171   2.287480   2.923809
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.166851    0.384745    0.004156
     2          8           0       -1.172850   -0.248014    0.005682
     3          7           0        1.075474   -0.154587   -0.058094
     4          1           0        1.858601    0.413268    0.180155
     5          1           0        1.157484   -1.131220    0.140399
     6          1           0       -0.160499    1.475700    0.015711
---------------------------------------------------------------------
Rotational constants (GHZ):     74.1372888     11.6647278     10.1158910
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.1075844788 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

```
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
               (A) (A) (A)
 Harris functional with IExCor=  205 diagonalized for initial guess.
 ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
 HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 ints in memory in canonical form, NReq=1726457.
 SCF Done:  E(RHF) =  -168.930294247     A.U. after   13 cycles
             Convg  =    0.6349D-08             -V/T =  2.0020
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.002559460   -0.002353792   -0.002599705
      2        8          -0.002870535    0.001578235    0.005951703
      3        7           0.000834488    0.004415144   -0.003792815
      4        1           0.000824723   -0.000555744    0.001180846
      5        1          -0.001730341   -0.002958308   -0.000646949
      6        1           0.000382205   -0.000125534   -0.000093080
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.005951703 RMS     0.002519884

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.006441487 RMS     0.002254142
 Search for a local minimum.
 Step number   7 out of a maximum of   25
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points    4    5    6    7
 DE= -1.19D-03 DEPred=-1.34D-03 R= 8.89D-01
 SS=  1.41D+00  RLast= 4.31D-01 DXNew= 1.2000D+00 1.2940D+00
 Trust test= 8.89D-01 RLast= 4.31D-01 DXMaxT set to 1.20D+00
 The second derivative matrix:
                        R1        R2        R3        R4        R5
          R1           0.96539
          R2           0.09598   0.31483
          R3           0.01591   0.01286   0.34959
          R4           0.02277   0.00845   0.00650   0.38137
          R5          -0.00403   0.00644   0.00694   0.01274   0.39486
          A1           0.06260   0.02895  -0.00817  -0.00276  -0.02061
          A2          -0.00335   0.00000   0.00506   0.00904   0.01702
          A3          -0.02532  -0.00750   0.00552   0.00705   0.01887
          A4           0.01900   0.01148  -0.00104  -0.00237  -0.00975
          A5          -0.01406   0.01346   0.00130   0.00655   0.01045
          A6          -0.00253   0.00208   0.00085   0.00016   0.00012
          D1          -0.00151   0.00185   0.00165  -0.00215  -0.00082
          D2           0.00740   0.02505   0.00307   0.00407   0.00324
          D3          -0.00628  -0.02191  -0.00215  -0.00537  -0.00502
          D4           0.00263   0.00129  -0.00074   0.00085  -0.00096
                         A1        A2        A3        A4        A5
          A1           0.17520
          A2          -0.08661   0.12498
          A3          -0.08930  -0.03238   0.13851
          A4           0.02295  -0.00982  -0.01025   0.13744
          A5          -0.02085   0.00698   0.01485  -0.03552   0.14103
          A6           0.00379  -0.00202  -0.00041  -0.05207  -0.04956
          D1           0.00900  -0.00048   0.00894   0.00060   0.00329
          D2           0.01132  -0.00358   0.01465  -0.00138   0.00795
          D3          -0.01309   0.00178  -0.01228  -0.00007  -0.00093
          D4          -0.01077  -0.00132  -0.00657  -0.00205   0.00373
                         A6        D1        D2        D3        D4
          A6           0.06107
          D1          -0.00732   0.03169
          D2           0.00548   0.02590   0.03829
          D3          -0.00536  -0.01854  -0.02569   0.02894
          D4           0.00744  -0.02433  -0.01330   0.02179   0.03282
 Use linear search instead of GDIIS.
     Eigenvalues ---    0.01185   0.02355   0.09134   0.14781   0.16017
     Eigenvalues ---    0.16961   0.25685   0.31186   0.34942   0.37339
     Eigenvalues ---    0.41469   0.988151000.000001000.000001000.00000
 RFO step:  Lambda=-3.28162360D-04 EMin= 1.18519687D-02
 Quartic linear search produced a step of -0.07832.
 Iteration  1 RMS(Cart)=  0.01631424 RMS(Int)=  0.00069387
 Iteration  2 RMS(Cart)=  0.00053174 RMS(Int)=  0.00048173
```

```
Iteration  3 RMS(Cart)=  0.00000011 RMS(Int)=  0.00048173
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.24585   0.00644  -0.00037   0.00584   0.00547   2.25132
   R2        2.56204   0.00151   0.00117  -0.00728  -0.00611   2.55594
   R3        2.06176  -0.00020  -0.00008  -0.00050  -0.00058   2.06118
   R4        1.88263  -0.00121   0.00010  -0.00438  -0.00428   1.87836
   R5        1.88967  -0.00294  -0.00004  -0.00678  -0.00682   1.88285
   A1        2.16990   0.00301  -0.00008   0.00860   0.00852   2.17842
   A2        2.13803  -0.00116  -0.00081   0.00182   0.00102   2.13904
   A3        1.97461  -0.00182   0.00093  -0.01022  -0.00930   1.96531
   A4        2.07439   0.00149  -0.00208   0.02218   0.01909   2.09348
   A5        2.04267  -0.00032  -0.00099   0.01036   0.00836   2.05103
   A6        2.03170  -0.00008  -0.00174   0.01516   0.01229   2.04399
   D1       -2.86814   0.00004   0.02140  -0.03975  -0.01857  -2.88672
   D2       -0.27895   0.00204   0.01283   0.05427   0.06732  -0.21163
   D3        0.31139  -0.00086   0.01963  -0.04566  -0.02625   0.28514
   D4        2.90059   0.00115   0.01106   0.04837   0.05964   2.96023
         Item               Value     Threshold  Converged?
Maximum Force            0.006441     0.000450     NO
RMS     Force            0.002254     0.000300     NO
Maximum Displacement     0.039860     0.001800     NO
RMS     Displacement     0.016324     0.001200     NO
Predicted change in Energy=-1.763945D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.089743    0.027104    0.050146
     2          8           0       -0.077471    0.184057    1.219211
     3          7           0        1.278911    0.147724   -0.582867
     4          1           0        1.308646    0.217367   -1.573964
     5          1           0        2.030399    0.561191   -0.075870
     6          1           0       -0.716597   -0.263792   -0.624302
---------------------------------------------------------------------
                    Distance matrix (angstroms):
                    1          2          3          4          5
    1  C    0.000000
    2  O    1.191347   0.000000
    3  N    1.352544   2.255788   0.000000
    4  H    2.039524   3.118374   0.993985   0.000000
    5  H    2.016748   2.502515   0.996361   1.698066   0.000000
    6  H    1.090727   2.001896   2.037919   2.288009   2.920165
                    6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.164917    0.382371    0.001158
     2          8           0       -1.177344   -0.245534    0.006940
     3          7           0        1.075894   -0.153647   -0.048333
     4          1           0        1.867720    0.407385    0.166751
     5          1           0        1.159851   -1.134800    0.103407
     6          1           0       -0.150578    1.472994    0.005708
---------------------------------------------------------------------
Rotational constants (GHZ):     74.9715522     11.6163506     10.0843580
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.0822306361 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Harris functional with IExCor=  205 diagonalized for initial guess.
```

```
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.930526700     A.U. after   13 cycles
           Convg  =    0.1443D-08             -V/T =  2.0020
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
     1        6          -0.000177895   -0.001266045   -0.000538013
     2        8          -0.000762099    0.000342230    0.000965618
     3        7           0.000659913    0.002233844   -0.000922585
     4        1           0.000158635   -0.000602573   -0.000373838
     5        1           0.000638633   -0.000711126    0.000406563
     6        1          -0.000517187    0.000003670    0.000462253
-------------------------------------------------------------------
Cartesian Forces:  Max     0.002233844 RMS     0.000813738

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.001779693 RMS     0.000725125
Search for a local minimum.
Step number   8 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points    4    5    6    7    8
DE= -2.32D-04 DEPred=-1.76D-04 R= 1.32D+00
SS=  1.41D+00  RLast= 1.00D-01 DXNew= 2.0182D+00 3.0000D-01
Trust test= 1.32D+00 RLast= 1.00D-01 DXMaxT set to 1.20D+00
The second derivative matrix:
                       R1        R2        R3        R4        R5
          R1           0.96843
          R2           0.06413   0.31327
          R3           0.01294   0.01534   0.35013
          R4           0.01165   0.01634   0.00821   0.38709
          R5          -0.02298   0.02423   0.01022   0.02386   0.41612
          A1           0.06291   0.01714  -0.00905  -0.00629  -0.02651
          A2           0.01039   0.00043   0.00393   0.00599   0.00979
          A3          -0.04520   0.00340   0.00812   0.01637   0.03713
          A4           0.01458   0.00055  -0.00180  -0.00502  -0.01351
          A5          -0.02846   0.01588   0.00264   0.01114   0.02018
          A6          -0.01200  -0.00049   0.00127   0.00162   0.00393
          D1           0.00350   0.00419   0.00168  -0.00221  -0.00171
          D2          -0.00231   0.01748   0.00315   0.00423   0.00486
          D3           0.00134  -0.01820  -0.00248  -0.00643  -0.00783
          D4          -0.00447  -0.00492  -0.00101   0.00000  -0.00126
                       A1        A2        A3        A4        A5
          A1           0.17453
          A2          -0.08199   0.12653
          A3          -0.09675  -0.03568   0.15384
          A4           0.02059  -0.00529  -0.01535   0.13451
          A5          -0.02645   0.00588   0.02160  -0.03986   0.14347
          A6          -0.00007  -0.00105   0.00140  -0.05537  -0.04972
          D1           0.01147  -0.00055   0.00958   0.00205   0.00382
          D2           0.00745   0.00048   0.01462  -0.00587   0.00568
          D3          -0.01022  -0.00085  -0.01403   0.00325  -0.00012
          D4          -0.01425   0.00018  -0.00898  -0.00467   0.00174
                       A6        D1        D2        D3        D4
          A6           0.05990
          D1          -0.00673   0.03220
          D2           0.00260   0.02806   0.03415
          D3          -0.00365  -0.02024  -0.02327   0.02788
          D4           0.00568  -0.02439  -0.01717   0.02485   0.03207
Use linear search instead of GDIIS.
    Eigenvalues ---    0.00839   0.01656   0.09508   0.14663   0.15977
    Eigenvalues ---    0.17630   0.26218   0.30609   0.34931   0.37329
    Eigenvalues ---    0.45597   0.986021000.000001000.000001000.00000
RFO step:  Lambda=-1.15158270D-04 EMin= 8.38719809D-03
Quartic linear search produced a step of  0.56224.
Iteration  1 RMS(Cart)=  0.02034949 RMS(Int)=  0.00172391
Iteration  2 RMS(Cart)=  0.00091668 RMS(Int)=  0.00147667
Iteration  3 RMS(Cart)=  0.00000059 RMS(Int)=  0.00147667
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
   R1        2.25132   0.00110   0.00307  -0.00083   0.00224   2.25356
```

```
   R2        2.55594   0.00178  -0.00343   0.00206  -0.00137   2.55457
   R3        2.06118   0.00010  -0.00033   0.00008  -0.00024   2.06093
   R4        1.87836   0.00034  -0.00240   0.00092  -0.00149   1.87687
   R5        1.88285   0.00039  -0.00383   0.00288  -0.00096   1.88189
   A1        2.17842   0.00038   0.00479  -0.00176   0.00302   2.18144
   A2        2.13904  -0.00089   0.00057  -0.00480  -0.00424   2.13481
   A3        1.96531   0.00052  -0.00523   0.00657   0.00134   1.96665
   A4        2.09348   0.00023   0.01074   0.01109   0.01863   2.11211
   A5        2.05103   0.00030   0.00470   0.01094   0.01244   2.06347
   A6        2.04399   0.00003   0.00691   0.01112   0.01466   2.05865
   D1       -2.88672  -0.00034  -0.01044  -0.05487  -0.06580  -2.95251
   D2       -0.21163   0.00096   0.03785   0.02462   0.06294  -0.14869
   D3        0.28514  -0.00068  -0.01476  -0.05522  -0.07046   0.21469
   D4        2.96023   0.00062   0.03353   0.02427   0.05828   3.01851
        Item               Value     Threshold  Converged?
Maximum Force            0.001780     0.000450     NO
RMS     Force            0.000725     0.000300     NO
Maximum Displacement     0.059511     0.001800     NO
RMS     Displacement     0.020079     0.001200     NO
Predicted change in Energy=-8.965410D-05
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.087365    0.030975    0.050923
     2          8           0       -0.080433    0.176057    1.222645
     3          7           0        1.269961    0.179215   -0.586966
     4          1           0        1.317123    0.201911   -1.578783
     5          1           0        2.038072    0.552156   -0.074473
     6          1           0       -0.718458   -0.266663   -0.620991
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.192533   0.000000
    3  N    1.351818   2.257934   0.000000
    4  H    2.048772   3.130787   0.993197   0.000000
    5  H    2.023021   2.512375   0.995855   1.704520   0.000000
    6  H    1.090599   2.000517   2.038081   2.297937   2.927047
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.165103    0.381570    0.001020
     2          8           0       -1.179531   -0.245370    0.005391
     3          7           0        1.076142   -0.152695   -0.034796
     4          1           0        1.879831    0.409021    0.123322
     5          1           0        1.167746   -1.138728    0.070439
     6          1           0       -0.153709    1.472109    0.000560
---------------------------------------------------------------------
Rotational constants (GHZ):     75.3832142     11.5842615     10.0549482
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.0373172306 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
```

```
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 ints in memory in canonical form, NReq=1726457.
 SCF Done:  E(RHF) =  -168.930641286     A.U. after   13 cycles
            Convg  =    0.2327D-08             -V/T =  2.0020
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000111910   -0.001057329   -0.000211220
      2        8           0.000346103    0.000281116   -0.000559947
      3        7          -0.000463562    0.001041240    0.001076010
      4        1          -0.000236039   -0.000351693   -0.000400646
      5        1           0.000450139   -0.000161086    0.000135333
      6        1          -0.000208551    0.000247753   -0.000039530
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.001076010 RMS     0.000518414

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000568430 RMS     0.000392872
 Search for a local minimum.
 Step number   9 out of a maximum of   25
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    5    6    7    8    9
 DE= -1.15D-04 DEPred=-8.97D-05 R= 1.28D+00
 SS=  1.41D+00  RLast= 1.32D-01 DXNew= 2.0182D+00 3.9582D-01
 Trust test= 1.28D+00 RLast= 1.32D-01 DXMaxT set to 1.20D+00
 The second derivative matrix:
                           R1        R2        R3        R4        R5
           R1           0.97584
           R2           0.08899   0.33452
           R3           0.01237   0.01448   0.35064
           R4           0.01099   0.01201   0.00896   0.38770
           R5          -0.01953   0.01867   0.01117   0.02405   0.41464
           A1           0.06914   0.03212  -0.00858  -0.00545  -0.02337
           A2          -0.00142  -0.01118   0.00361   0.00663   0.01038
           A3          -0.04410  -0.00343   0.00832   0.01533   0.03448
           A4           0.02195   0.01012  -0.00277  -0.00708  -0.01547
           A5          -0.03082   0.01029   0.00329   0.01165   0.02039
           A6          -0.01526  -0.00469   0.00152   0.00162   0.00407
           D1          -0.00245   0.00047   0.00243  -0.00006   0.00119
           D2          -0.00501   0.01725   0.00308   0.00371   0.00518
           D3           0.00455  -0.01647  -0.00268  -0.00644  -0.00855
           D4           0.00199   0.00032  -0.00203  -0.00267  -0.00456
                           A1        A2        A3        A4        A5
           A1           0.18007
           A2          -0.09011   0.13355
           A3          -0.09559  -0.03365   0.15046
           A4           0.02421  -0.00919  -0.01701   0.13912
           A5          -0.02665   0.00729   0.02060  -0.04234   0.14390
           A6          -0.00100   0.00020   0.00039  -0.05707  -0.04992
           D1           0.00857   0.00107   0.01236  -0.00083   0.00619
           D2           0.00700   0.00010   0.01362  -0.00635   0.00470
           D3          -0.00959  -0.00096  -0.01333   0.00440   0.00024
           D4          -0.01116  -0.00194  -0.01208  -0.00113  -0.00125
                           A6        D1        D2        D3        D4
           A6           0.05907
           D1          -0.00513   0.03336
           D2           0.00075   0.02887   0.03165
           D3          -0.00243  -0.02135  -0.02107   0.02623
           D4           0.00344  -0.02584  -0.01829   0.02650   0.03405
       Eigenvalues ---    0.00467   0.01636   0.09791   0.14458   0.16269
       Eigenvalues ---    0.17856   0.26215   0.33191   0.35005   0.37331
       Eigenvalues ---    0.45132   1.001261000.000001000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     9    8
 RFO step:  Lambda=-7.40724774D-06.
 DIIS coeffs:      1.50476     -0.50476
 Iteration  1 RMS(Cart)=  0.01604672 RMS(Int)=  0.00143480
 Iteration  2 RMS(Cart)=  0.00060080 RMS(Int)=  0.00131261
 Iteration  3 RMS(Cart)=  0.00000023 RMS(Int)=  0.00131261
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                  (DIIS)     (GDIIS)  (Total)
      R1        2.25356  -0.00056   0.00113  -0.00023   0.00090   2.25446
      R2        2.55457  -0.00054  -0.00069  -0.00731  -0.00800   2.54657
      R3        2.06093   0.00011  -0.00012   0.00030   0.00018   2.06111
      R4        1.87687   0.00038  -0.00075   0.00034  -0.00041   1.87646
```

```
   R5        1.88189   0.00036  -0.00048  -0.00014  -0.00062   1.88127
   A1        2.18144  -0.00057   0.00152  -0.00256  -0.00106   2.18038
   A2        2.13481   0.00019  -0.00214   0.00357   0.00141   2.13622
   A3        1.96665   0.00040   0.00068  -0.00079  -0.00013   1.96651
   A4        2.11211  -0.00043   0.00941   0.00104   0.00755   2.11967
   A5        2.06347   0.00043   0.00628   0.00597   0.00936   2.07283
   A6        2.05865   0.00013   0.00740   0.00449   0.00892   2.06757
   D1       -2.95251   0.00002  -0.03321  -0.02471  -0.05822  -3.01073
   D2       -0.14869   0.00050   0.03177   0.01454   0.04661  -0.10208
   D3        0.21469  -0.00051  -0.03556  -0.03475  -0.07061   0.14408
   D4        3.01851  -0.00003   0.02942   0.00450   0.03421   3.05273
       Item               Value     Threshold  Converged?
Maximum Force            0.000568     0.000450     NO
RMS     Force            0.000393     0.000300     NO
Maximum Displacement     0.046483     0.001800     NO
RMS     Displacement     0.015995     0.001200     NO
Predicted change in Energy=-3.169411D-05
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.087392    0.032016    0.050666
     2          8           0       -0.078227    0.168097    1.224260
     3          7           0        1.261609    0.203813   -0.587836
     4          1           0        1.320004    0.184943   -1.578918
     5          1           0        2.040802    0.548788   -0.073128
     6          1           0       -0.717950   -0.264006   -0.622689
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.193010   0.000000
    3  N    1.347584   2.253914   0.000000
    4  H    2.048966   3.132594   0.992981   0.000000
    5  H    2.024397   2.513647   0.995526   1.708606   0.000000
    6  H    1.090693   2.001795   2.034385   2.295470   2.928030
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.163640    0.381700   -0.000033
     2          8           0       -1.178915   -0.244776    0.003905
     3          7           0        1.072970   -0.153287   -0.023899
     4          1           0        1.883386    0.410182    0.084452
     5          1           0        1.168914   -1.141472    0.049288
     6          1           0       -0.149928    1.472304    0.002511
---------------------------------------------------------------------
Rotational constants (GHZ):     75.5082174     11.6188784     10.0759715
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.1042173462 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
```

```
       I1Cent=           4 NGrid=           0.
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.930677463     A.U. after   12 cycles
            Convg  =    0.9065D-08             -V/T =  2.0020
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
     1        6          -0.001678974   -0.000194841    0.001031228
     2        8          -0.000083414   -0.000131444   -0.000406031
     3        7           0.001645334    0.000665015   -0.000702438
     4        1          -0.000035610   -0.000181146   -0.000227822
     5        1           0.000397300   -0.000058959    0.000112078
     6        1          -0.000244637   -0.000098624    0.000192986
-------------------------------------------------------------------
Cartesian Forces:  Max     0.001678974 RMS     0.000671603

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.002190654 RMS     0.000606728
Search for a local minimum.
Step number  10 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swaping is turned off.
Update second derivatives using D2CorX and points    5    7    8    9   10
DE= -3.62D-05 DEPred=-3.17D-05 R= 1.14D+00
SS=  1.41D+00  RLast= 1.10D-01 DXNew= 2.0182D+00 3.2877D-01
Trust test= 1.14D+00 RLast= 1.10D-01 DXMaxT set to 1.20D+00
The second derivative matrix:
                       R1        R2        R3        R4        R5
          R1           0.95337
          R2           0.07970   0.44194
          R3           0.01021   0.01660   0.35037
          R4           0.01079   0.01350   0.00864   0.38685
          R5          -0.01744   0.02873   0.01126   0.02357   0.41495
          A1           0.05153   0.05029  -0.00958  -0.00510  -0.01982
          A2           0.00481  -0.02827   0.00374   0.00626   0.00795
          A3          -0.03464  -0.00008   0.00877   0.01416   0.03279
          A4           0.01817   0.01001  -0.00279  -0.00603  -0.01398
          A5          -0.02758   0.00631   0.00312   0.01067   0.01872
          A6          -0.01577  -0.00785   0.00110   0.00070   0.00306
          D1          -0.00109  -0.00686   0.00226  -0.00039  -0.00017
          D2          -0.00001   0.00057   0.00254   0.00170   0.00178
          D3           0.00510  -0.00273  -0.00181  -0.00481  -0.00647
          D4           0.00618   0.00470  -0.00154  -0.00271  -0.00453
                         A1        A2        A3        A4        A5
          A1           0.17179
          A2          -0.08922   0.13554
          A3          -0.08795  -0.03689   0.14490
          A4           0.02109  -0.00822  -0.01384   0.13764
          A5          -0.02519   0.00724   0.01819  -0.04101   0.14306
          A6          -0.00175   0.00099  -0.00074  -0.05622  -0.05043
          D1           0.00761   0.00226   0.01199  -0.00099   0.00651
          D2           0.00740   0.00106   0.00937  -0.00397   0.00375
          D3          -0.00675  -0.00298  -0.01144   0.00296   0.00078
          D4          -0.00697  -0.00418  -0.01405  -0.00001  -0.00198
                         A6        D1        D2        D3        D4
          A6           0.05859
          D1          -0.00493   0.03411
          D2          -0.00041   0.03075   0.03107
          D3          -0.00137  -0.02255  -0.02046   0.02522
          D4           0.00315  -0.02591  -0.02013   0.02731   0.03308
    Eigenvalues ---    0.00256   0.01555   0.10179   0.14356   0.16239
    Eigenvalues ---    0.17757   0.25150   0.34812   0.37302   0.42008
    Eigenvalues ---    0.47063   0.974441000.000001000.000001000.00000
En-DIIS/RFO-DIIS IScMMF=        0 using points:    10    9    8
RFO step:  Lambda=-9.42295308D-06.
DIIS coeffs:      0.76490      0.62546     -0.39035
Iteration  1 RMS(Cart)=  0.00495393 RMS(Int)=  0.00104826
Iteration  2 RMS(Cart)=  0.00005295 RMS(Int)=  0.00104694
Iteration  3 RMS(Cart)=  0.00000002 RMS(Int)=  0.00104694
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                  (DIIS)     (GDIIS)  (Total)
   R1        2.25446  -0.00040   0.00066  -0.00105  -0.00039   2.25407
   R2        2.54657   0.00219   0.00135   0.00178   0.00312   2.54969
   R3        2.06111   0.00009  -0.00014   0.00011  -0.00003   2.06108
   R4        1.87646   0.00023  -0.00048   0.00044  -0.00004   1.87642
   R5        1.88127   0.00035  -0.00023   0.00020  -0.00003   1.88124
   A1        2.18038   0.00002   0.00143  -0.00153  -0.00011   2.18027
   A2        2.13622  -0.00033  -0.00198   0.00104  -0.00094   2.13527
```

```
   A3        1.96651   0.00030   0.00055   0.00051   0.00106   1.96757
   A4        2.11967  -0.00016   0.00550  -0.00181   0.00137   2.12104
   A5        2.07283   0.00024   0.00266   0.00191   0.00225   2.07508
   A6        2.06757  -0.00002   0.00362   0.00087   0.00214   2.06970
   D1       -3.01073  -0.00019  -0.01200  -0.00534  -0.01754  -3.02827
   D2       -0.10208   0.00010   0.01361  -0.00037   0.01344  -0.08864
   D3        0.14408  -0.00008  -0.01090  -0.00684  -0.01794   0.12613
   D4        3.05273   0.00021   0.01471  -0.00187   0.01303   3.06576
        Item               Value     Threshold  Converged?
Maximum Force            0.002191     0.000450     NO
RMS     Force            0.000607     0.000300     NO
Maximum Displacement     0.014368     0.001800     NO
RMS     Displacement     0.004931     0.001200     NO
Predicted change in Energy=-1.198929D-05
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.086147    0.032990    0.050892
     2          8           0       -0.078957    0.165583    1.224750
     3          7           0        1.260573    0.211417   -0.588893
     4          1           0        1.322100    0.180761   -1.579469
     5          1           0        2.043072    0.547306   -0.073222
     6          1           0       -0.719303   -0.264405   -0.621703
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.192804   0.000000
    3  N    1.349236   2.255159   0.000000
    4  H    2.051218   3.134778   0.992958   0.000000
    5  H    2.027186   2.516635   0.995512   1.709660   0.000000
    6  H    1.090678   2.001080   2.036515   2.298437   2.930943
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.164614    0.381836    0.000185
     2          8           0       -1.179243   -0.245301    0.003354
     3          7           0        1.073899   -0.153034   -0.020726
     4          1           0        1.885080    0.411865    0.073301
     5          1           0        1.172017   -1.141686    0.042382
     6          1           0       -0.152766    1.472449    0.001461
---------------------------------------------------------------------
Rotational constants (GHZ):     75.4819700     11.6043865     10.0629780
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.0719938124 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.930688926     A.U. after   11 cycles
           Convg  =    0.3740D-08             -V/T =  2.0020
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
```

```
Number     Number              X              Y              Z
---------------------------------------------------------------------
     1        6          -0.000155287   -0.000140516    0.000249560
     2        8          -0.000002949   -0.000008544   -0.000197413
     3        7          -0.000030355    0.000282709    0.000029610
     4        1          -0.000026042   -0.000122794   -0.000162740
     5        1           0.000263191   -0.000018197    0.000093185
     6        1          -0.000048557    0.000007343   -0.000012202
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000282709 RMS     0.000139444

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.000249005 RMS     0.000126228
Search for a local minimum.
Step number  11 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swaping is turned off.
Update second derivatives using D2CorX and points    5    7    8    9   10
                                                    11
DE= -1.15D-05 DEPred=-1.20D-05 R= 9.56D-01
SS=  1.41D+00  RLast= 3.17D-02 DXNew= 2.0182D+00 9.5036D-02
Trust test= 9.56D-01 RLast= 3.17D-02 DXMaxT set to 1.20D+00
The second derivative matrix:
                       R1        R2        R3        R4        R5
          R1           0.93923
          R2           0.06740   0.52510
          R3           0.00695   0.01372   0.34927
          R4           0.00840   0.00383   0.00710   0.38430
          R5          -0.01715   0.01277   0.00975   0.02062   0.41130
          A1           0.03718   0.02916  -0.01400  -0.01002  -0.02290
          A2           0.00792  -0.03435   0.00497   0.00875   0.01112
          A3          -0.03358   0.02555   0.00959   0.01417   0.03145
          A4           0.02224   0.01686  -0.00125  -0.00371  -0.01142
          A5          -0.02570   0.00931   0.00317   0.00988   0.01673
          A6          -0.01563  -0.01920   0.00024  -0.00088   0.00092
          D1          -0.00199  -0.00978   0.00216  -0.00004   0.00067
          D2           0.00123   0.00059   0.00254   0.00123   0.00051
          D3           0.00801   0.00274  -0.00067  -0.00319  -0.00468
          D4           0.01123   0.01312  -0.00029  -0.00192  -0.00484
                       A1        A2        A3        A4        A5
          A1           0.15566
          A2          -0.08294   0.13612
          A3          -0.08717  -0.04034   0.15003
          A4           0.02673  -0.01095  -0.01462   0.13572
          A5          -0.02520   0.00673   0.01884  -0.04062   0.14301
          A6          -0.00325   0.00346  -0.00225  -0.05504  -0.05138
          D1           0.00719   0.00244   0.01097  -0.00106   0.00685
          D2           0.00708   0.00091   0.00968  -0.00361   0.00391
          D3          -0.00209  -0.00452  -0.01191   0.00135   0.00068
          D4          -0.00221  -0.00605  -0.01319  -0.00121  -0.00226
                       A6        D1        D2        D3        D4
          A6           0.05800
          D1          -0.00423   0.03404
          D2          -0.00086   0.03115   0.03144
          D3          -0.00056  -0.02269  -0.02070   0.02427
          D4           0.00281  -0.02558  -0.02041   0.02626   0.03144
    Eigenvalues ---    0.00208   0.01400   0.10111   0.14160   0.15790
    Eigenvalues ---    0.17784   0.25299   0.34802   0.37273   0.43650
    Eigenvalues ---    0.52736   0.956631000.000001000.000001000.00000
En-DIIS/RFO-DIIS IScMMF=        0 using points:    11   10    9    8
RFO step:  Lambda=-9.52084674D-07.
DIIS coeffs:      1.39600     -0.12078     -0.18568     -0.08953
Iteration  1 RMS(Cart)=  0.00819842 RMS(Int)=  0.00085423
Iteration  2 RMS(Cart)=  0.00015530 RMS(Int)=  0.00084054
Iteration  3 RMS(Cart)=  0.00000003 RMS(Int)=  0.00084054
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                  (DIIS)     (GDIIS)  (Total)
   R1        2.25407  -0.00019   0.00029  -0.00025   0.00005   2.25412
   R2        2.54969   0.00022  -0.00109  -0.00003  -0.00112   2.54857
   R3        2.06108   0.00004   0.00002   0.00009   0.00011   2.06119
   R4        1.87642   0.00016  -0.00026   0.00025  -0.00001   1.87641
   R5        1.88124   0.00025  -0.00027   0.00052   0.00025   1.88150
   A1        2.18027   0.00003  -0.00006   0.00064   0.00056   2.18083
   A2        2.13527  -0.00003  -0.00037   0.00021  -0.00017   2.13510
   A3        1.96757   0.00001   0.00050  -0.00085  -0.00036   1.96721
   A4        2.12104  -0.00010   0.00429  -0.00032   0.00210   2.12315
   A5        2.07508   0.00013   0.00458   0.00060   0.00331   2.07839
   A6        2.06970   0.00000   0.00461  -0.00007   0.00266   2.07236
   D1       -3.02827  -0.00007  -0.02886  -0.00184  -0.03081  -3.05908
   D2       -0.08864   0.00011   0.02379  -0.00065   0.02326  -0.06538
   D3        0.12613  -0.00011  -0.03285  -0.00139  -0.03435   0.09178
   D4        3.06576   0.00007   0.01980  -0.00020   0.01972   3.08548
         Item               Value     Threshold  Converged?
Maximum Force            0.000249     0.000450     YES
RMS     Force            0.000126     0.000300     YES
Maximum Displacement     0.024099     0.001800     NO
```

```
RMS     Displacement     0.008175     0.001200     NO
Predicted change in Energy=-6.314749D-06
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.085747    0.034284    0.051059
     2          8           0       -0.078848    0.161201    1.225641
     3          7           0        1.257018    0.224169   -0.589966
     4          1           0        1.323846    0.172378   -1.579314
     5          1           0        2.045096    0.545237   -0.073093
     6          1           0       -0.719228   -0.263618   -0.621972
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.192830   0.000000
    3  N    1.348646   2.254980   0.000000
    4  H    2.051846   3.136152   0.992953   0.000000
    5  H    2.028679   2.518995   0.995645   1.711118   0.000000
    6  H    1.090734   2.001058   2.035807   2.297987   2.932064
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.164527    0.381548    0.000155
     2          8           0       -1.179478   -0.245121    0.002428
     3          7           0        1.073552   -0.153028   -0.015174
     4          1           0        1.886387    0.413159    0.053303
     5          1           0        1.174078   -1.142494    0.031290
     6          1           0       -0.152348    1.472213    0.001274
---------------------------------------------------------------------
Rotational constants (GHZ):     75.5670608     11.6040679     10.0619683
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.0757293806 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.930696283     A.U. after   11 cycles
            Convg  =    0.5431D-08             -V/T =  2.0020
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
---------------------------------------------------------------------
```

```
     1        6          -0.000310798   -0.000126699    0.000181336
     2        8           0.000035907    0.000014905   -0.000077098
     3        7           0.000244405    0.000242887   -0.000040387
     4        1           0.000012093   -0.000057806   -0.000046174
     5        1           0.000043507   -0.000067680   -0.000016335
     6        1          -0.000025114   -0.000005607   -0.000001342
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000310798 RMS     0.000126133

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.000325986 RMS     0.000095286
Search for a local minimum.
Step number  12 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swaping is turned off.
Update second derivatives using D2CorX and points    5    7    8    9   10
                                                    11   12
DE= -7.36D-06 DEPred=-6.31D-06 R= 1.17D+00
SS=  1.41D+00  RLast= 5.55D-02 DXNew= 2.0182D+00 1.6658D-01
Trust test= 1.17D+00 RLast= 5.55D-02 DXMaxT set to 1.20D+00
The second derivative matrix:
                       R1        R2        R3        R4        R5
          R1           0.94304
          R2           0.05612   0.51653
          R3           0.00692   0.01061   0.34866
          R4           0.00578  -0.00008   0.00589   0.38301
          R5          -0.02566   0.01051   0.00816   0.02089   0.41691
          A1           0.03084   0.01793  -0.01574  -0.01233  -0.02600
          A2           0.01209  -0.02945   0.00550   0.00883   0.01017
          A3          -0.03058   0.03265   0.00999   0.01494   0.03353
          A4           0.02229   0.02045  -0.00001  -0.00154  -0.00961
          A5          -0.02714   0.01121   0.00324   0.01090   0.01981
          A6          -0.01692  -0.02372  -0.00089  -0.00298  -0.00163
          D1           0.00077  -0.00991   0.00246  -0.00028  -0.00096
          D2           0.00235   0.00048   0.00275   0.00133   0.00099
          D3           0.00642   0.00552  -0.00026  -0.00201  -0.00331
          D4           0.00801   0.01591   0.00003  -0.00040  -0.00136
                       A1        A2        A3        A4        A5
          A1           0.14546
          A2          -0.07867   0.13511
          A3          -0.08188  -0.04365   0.14730
          A4           0.02801  -0.01111  -0.01428   0.13290
          A5          -0.02384   0.00511   0.01885  -0.04080   0.14464
          A6          -0.00596   0.00533  -0.00198  -0.05310  -0.05201
          D1           0.00786   0.00222   0.01016  -0.00117   0.00636
          D2           0.00890   0.00027   0.00939  -0.00339   0.00426
          D3          -0.00226  -0.00422  -0.01157  -0.00017   0.00050
          D4          -0.00123  -0.00617  -0.01234  -0.00239  -0.00159
                       A6        D1        D2        D3        D4
          A6           0.05714
          D1          -0.00401   0.03451
          D2          -0.00139   0.03150   0.03083
          D3           0.00091  -0.02323  -0.02049   0.02370
          D4           0.00353  -0.02624  -0.02116   0.02644   0.03152
    Eigenvalues ---    0.00128   0.01289   0.10155   0.13704   0.15607
    Eigenvalues ---    0.17968   0.24258   0.34839   0.37251   0.43990
    Eigenvalues ---    0.52262   0.956551000.000001000.000001000.00000
En-DIIS/RFO-DIIS IScMMF=        0 using points:    12   11   10    9    8
RFO step:  Lambda=-4.52721689D-07.
DIIS coeffs:      1.00625      0.30700     -0.16072     -0.10654     -0.04599
Iteration  1 RMS(Cart)=  0.00481959 RMS(Int)=  0.00064690
Iteration  2 RMS(Cart)=  0.00005539 RMS(Int)=  0.00064461
Iteration  3 RMS(Cart)=  0.00000001 RMS(Int)=  0.00064461
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (DIIS)     (GDIIS)  (Total)
   R1        2.25412  -0.00008   0.00012  -0.00010   0.00002   2.25414
   R2        2.54857   0.00033  -0.00031   0.00007  -0.00025   2.54833
   R3        2.06119   0.00002   0.00001   0.00001   0.00002   2.06121
   R4        1.87641   0.00005  -0.00014   0.00002  -0.00012   1.87629
   R5        1.88150   0.00000  -0.00015  -0.00007  -0.00022   1.88128
   A1        2.18083  -0.00006  -0.00005  -0.00006  -0.00012   2.18071
   A2        2.13510   0.00001  -0.00028   0.00044   0.00016   2.13526
   A3        1.96721   0.00004   0.00037  -0.00038  -0.00002   1.96720
   A4        2.12315  -0.00002   0.00245   0.00014   0.00116   2.12431
   A5        2.07839   0.00005   0.00273   0.00009   0.00138   2.07978
   A6        2.07236  -0.00002   0.00272  -0.00017   0.00111   2.07347
   D1       -3.05908  -0.00004  -0.01759  -0.00030  -0.01797  -3.07704
   D2       -0.06538   0.00007   0.01436   0.00022   0.01465  -0.05073
   D3        0.09178  -0.00005  -0.01985  -0.00012  -0.02004   0.07175
   D4        3.08548   0.00005   0.01211   0.00041   0.01259   3.09806
        Item               Value     Threshold  Converged?
Maximum Force            0.000326     0.000450     YES
RMS     Force            0.000095     0.000300     YES
Maximum Displacement     0.014515     0.001800     NO
RMS     Displacement     0.004811     0.001200     NO
Predicted change in Energy=-2.631838D-06
```

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.085379    0.035034    0.051061
     2          8           0       -0.078450    0.158891    1.226089
     3          7           0        1.254922    0.231850   -0.590754
     4          1           0        1.325155    0.167733   -1.579079
     5          1           0        2.045967    0.543609   -0.072936
     6          1           0       -0.719341   -0.263466   -0.622025
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.192841   0.000000
    3  N    1.348516   2.254800   0.000000
    4  H    2.052319   3.136742   0.992890   0.000000
    5  H    2.029268   2.519646   0.995530   1.711525   0.000000
    6  H    1.090744   2.001163   2.035690   2.298228   2.932541
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.164564    0.381588    0.000095
     2          8           0       -1.179487   -0.245146    0.001917
     3          7           0        1.073389   -0.153041   -0.011819
     4          1           0        1.887087    0.413407    0.041682
     5          1           0        1.174752   -1.142741    0.024232
     6          1           0       -0.152279    1.472262    0.000910
---------------------------------------------------------------------
Rotational constants (GHZ):     75.5787156     11.6048898     10.0617677
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.0771784143 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on              energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.930699082     A.U. after   10 cycles
           Convg  =    0.8617D-08             -V/T =  2.0020
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
     1        6          -0.000194399   -0.000072572    0.000142732
     2        8          -0.000005258   -0.000001785   -0.000038373
     3        7           0.000127478    0.000142148   -0.000083271
     4        1           0.000015465   -0.000045595   -0.000059399
     5        1           0.000075606   -0.000020711    0.000030995
     6        1          -0.000018892   -0.000001485    0.000007317
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000194399 RMS     0.000082222

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
```

```
Internal  Forces:  Max     0.000253764 RMS     0.000073557
Search for a local minimum.
Step number  13 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swaping is turned off.
Update second derivatives using D2CorX and points    5    7    8    9   10
                                                    11   12   13
DE= -2.80D-06 DEPred=-2.63D-06 R= 1.06D+00
SS=  1.41D+00  RLast= 3.32D-02 DXNew= 2.0182D+00 9.9591D-02
Trust test= 1.06D+00 RLast= 3.32D-02 DXMaxT set to 1.20D+00
The second derivative matrix:
                      R1        R2        R3        R4        R5
          R1           0.91644
          R2           0.03948   0.49391
          R3           0.00368   0.00669   0.34785
          R4           0.00755  -0.00583   0.00478   0.38103
          R5          -0.01472   0.00854   0.00768   0.01962   0.41673
          A1           0.01636   0.00487  -0.01871  -0.01231  -0.01810
          A2           0.02052  -0.02225   0.00675   0.00829   0.00524
          A3          -0.01919   0.03983   0.01165   0.01435   0.02863
          A4           0.02216   0.02565   0.00119   0.00133  -0.00600
          A5          -0.02333   0.01603   0.00445   0.01078   0.01753
          A6          -0.01729  -0.02989  -0.00233  -0.00510  -0.00361
          D1          -0.00055  -0.00949   0.00247   0.00022  -0.00018
          D2           0.00075  -0.00118   0.00291   0.00086  -0.00027
          D3           0.00903   0.01051   0.00046  -0.00066  -0.00209
          D4           0.01033   0.01883   0.00090  -0.00002  -0.00218
                        A1        A2        A3        A4        A5
          A1           0.13948
          A2          -0.07507   0.13350
          A3          -0.07594  -0.04728   0.14245
          A4           0.03065  -0.01192  -0.01472   0.13004
          A5          -0.02130   0.00329   0.01730  -0.04154   0.14606
          A6          -0.00829   0.00678  -0.00176  -0.05069  -0.05297
          D1           0.00712   0.00256   0.01085  -0.00160   0.00661
          D2           0.00709   0.00128   0.01009  -0.00379   0.00524
          D3           0.00085  -0.00556  -0.01293  -0.00133  -0.00061
          D4           0.00082  -0.00683  -0.01369  -0.00352  -0.00199
                        A6        D1        D2        D3        D4
          A6           0.05639
          D1          -0.00373   0.03441
          D2          -0.00173   0.03175   0.03100
          D3           0.00232  -0.02352  -0.02057   0.02302
          D4           0.00432  -0.02618  -0.02132   0.02596   0.03082
     Eigenvalues ---    0.00092   0.01154   0.09876   0.13019   0.15633
     Eigenvalues ---    0.18091   0.23960   0.34905   0.37192   0.43486
     Eigenvalues ---    0.50523   0.923861000.000001000.000001000.00000
En-DIIS/RFO-DIIS IScMMF=        0 using points:    13   12   11   10    9
RFO step:  Lambda=-2.59538297D-07.
DIIS coeffs:      1.80592     -0.36678     -0.32077     -0.11576     -0.00260
Iteration  1 RMS(Cart)=  0.00810838 RMS(Int)=  0.00050253
Iteration  2 RMS(Cart)=  0.00015268 RMS(Int)=  0.00047972
Iteration  3 RMS(Cart)=  0.00000001 RMS(Int)=  0.00047972
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                  (DIIS)     (GDIIS)  (Total)
   R1        2.25414  -0.00004  -0.00001   0.00006   0.00006   2.25420
   R2        2.54833   0.00025  -0.00034   0.00003  -0.00031   2.54802
   R3        2.06121   0.00001   0.00006  -0.00004   0.00002   2.06123
   R4        1.87629   0.00006  -0.00011   0.00005  -0.00006   1.87623
   R5        1.88128   0.00007  -0.00007   0.00003  -0.00004   1.88124
   A1        2.18071   0.00000   0.00013   0.00001   0.00014   2.18085
   A2        2.13526  -0.00002  -0.00006   0.00008   0.00002   2.13528
   A3        1.96720   0.00002  -0.00005  -0.00009  -0.00014   1.96705
   A4        2.12431   0.00000   0.00204   0.00032   0.00129   2.12559
   A5        2.07978   0.00002   0.00286  -0.00025   0.00154   2.08132
   A6        2.07347  -0.00001   0.00234  -0.00001   0.00125   2.07472
   D1       -3.07704  -0.00003  -0.03024  -0.00034  -0.03060  -3.10765
   D2       -0.05073   0.00004   0.02373   0.00022   0.02399  -0.02674
   D3        0.07175  -0.00004  -0.03354  -0.00047  -0.03404   0.03771
   D4        3.09806   0.00003   0.02043   0.00009   0.02055   3.11862
         Item               Value     Threshold  Converged?
Maximum Force            0.000254     0.000450     YES
RMS     Force            0.000074     0.000300     YES
Maximum Displacement     0.024201     0.001800     NO
RMS     Displacement     0.008095     0.001200     NO
Predicted change in Energy=-2.359898D-06
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.084908    0.036333    0.051061
     2          8           0       -0.077808    0.154800    1.226830
     3          7           0        1.251468    0.244657   -0.592208
     4          1           0        1.327279    0.159699   -1.578515
     5          1           0        2.047242    0.541108   -0.072694
```

```
     6          1           0       -0.719459   -0.262945   -0.622119
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.192872   0.000000
    3  N    1.348353   2.254762   0.000000
    4  H    2.052857   3.137555   0.992857   0.000000
    5  H    2.029992   2.520682   0.995507   1.712109   0.000000
    6  H    1.090755   2.001210   2.035463   2.298360   2.933088
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.164581    0.381525    0.000049
     2          8           0       -1.179602   -0.245111    0.001008
     3          7           0        1.073267   -0.153032   -0.006220
     4          1           0        1.887906    0.413835    0.021903
     5          1           0        1.175681   -1.143075    0.012773
     6          1           0       -0.152154    1.472209    0.000502
---------------------------------------------------------------------
Rotational constants (GHZ):     75.6104424     11.6041670     10.0606372
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.0770187103 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Harris functional with IExCor=  205 diagonalized for initial guess.
ExpMin= 1.61D-01 ExpMax= 5.48D+03 ExpMxC= 8.25D+02 IAcc=1 IRadAn=         1 AccDes= 0.00D+00
HarFok:  IExCor=  205 AccDes= 0.00D+00 IRadAn=         1 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.930701781     A.U. after   11 cycles
           Convg  =    0.5166D-08             -V/T =  2.0020
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
---------------------------------------------------------------------
     1        6          -0.000143897   -0.000039483    0.000096828
     2        8           0.000004872   -0.000001891   -0.000032991
     3        7           0.000105043    0.000073287   -0.000067191
     4        1           0.000011944   -0.000020176   -0.000033435
     5        1           0.000035477   -0.000008782    0.000024396
     6        1          -0.000013439   -0.000002956    0.000012393
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000143897 RMS     0.000056577

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.000175124 RMS     0.000049451
Search for a local minimum.
```

```
Step number  14 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swaping is turned off.
Update second derivatives using D2CorX and points    7    8    9   10   11
                                                    12   13   14
DE= -2.70D-06 DEPred=-2.36D-06 R= 1.14D+00
SS=  1.41D+00  RLast= 5.57D-02 DXNew= 2.0182D+00 1.6700D-01
Trust test= 1.14D+00 RLast= 5.57D-02 DXMaxT set to 1.20D+00
The second derivative matrix:
                      R1        R2        R3        R4        R5
          R1           0.85138
          R2           0.08435   0.47990
          R3           0.00634   0.00613   0.34780
          R4           0.03027  -0.01822   0.00380   0.37338
          R5           0.02580  -0.01378   0.00600   0.00634   0.39363
          A1          -0.00996   0.02910  -0.01747  -0.00258  -0.00045
          A2           0.02883  -0.03099   0.00606   0.00456  -0.00148
          A3           0.00327   0.02374   0.01086   0.00684   0.01509
          A4          -0.00159   0.03952   0.00228   0.00981   0.00880
          A5          -0.02477   0.01603   0.00496   0.01141   0.01827
          A6           0.00077  -0.03930  -0.00345  -0.01133  -0.01441
          D1          -0.00886  -0.00504   0.00274   0.00275   0.00423
          D2          -0.00732   0.00200   0.00327   0.00370   0.00489
          D3           0.00821   0.01140   0.00051  -0.00031  -0.00164
          D4           0.00975   0.01844   0.00105   0.00063  -0.00098
                      A1        A2        A3        A4        A5
          A1           0.13047
          A2          -0.07298   0.13350
          A3          -0.06682  -0.05021   0.13449
          A4           0.02090  -0.00843  -0.00689   0.12095
          A5          -0.02146   0.00314   0.01734  -0.04219   0.14829
          A6          -0.00097   0.00445  -0.00767  -0.04397  -0.05429
          D1           0.00309   0.00391   0.01385  -0.00449   0.00657
          D2           0.00387   0.00250   0.01253  -0.00661   0.00564
          D3           0.00055  -0.00528  -0.01266  -0.00191  -0.00121
          D4           0.00133  -0.00669  -0.01398  -0.00403  -0.00214
                      A6        D1        D2        D3        D4
          A6           0.05287
          D1          -0.00174   0.03355
          D2           0.00011   0.03096   0.02985
          D3           0.00302  -0.02368  -0.02070   0.02301
          D4           0.00486  -0.02627  -0.02181   0.02598   0.03044
    Eigenvalues ---    0.00069   0.00969   0.09848   0.11680   0.15409
    Eigenvalues ---    0.17919   0.22712   0.34920   0.36976   0.39677
    Eigenvalues ---    0.48827   0.873691000.000001000.000001000.00000
En-DIIS/RFO-DIIS IScMMF=        0 using points:    14   13   12   11   10
RFO step:  Lambda=-8.91247810D-08.
DIIS coeffs:      1.55565     -0.42297     -0.14820      0.07945     -0.06393
Iteration  1 RMS(Cart)=  0.00530493 RMS(Int)=  0.00026117
Iteration  2 RMS(Cart)=  0.00006556 RMS(Int)=  0.00025315
Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00025315
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (DIIS)     (GDIIS)  (Total)
   R1        2.25420  -0.00003   0.00001  -0.00003  -0.00002   2.25418
   R2        2.54802   0.00018   0.00001   0.00000   0.00001   2.54803
   R3        2.06123   0.00000   0.00001  -0.00002  -0.00001   2.06122
   R4        1.87623   0.00004  -0.00005   0.00005   0.00000   1.87623
   R5        1.88124   0.00004  -0.00006   0.00007   0.00002   1.88125
   A1        2.18085  -0.00001   0.00005  -0.00009  -0.00005   2.18080
   A2        2.13528  -0.00001  -0.00003   0.00004   0.00001   2.13529
   A3        1.96705   0.00003  -0.00001   0.00005   0.00004   1.96710
   A4        2.12559   0.00001   0.00092   0.00013   0.00049   2.12609
   A5        2.08132   0.00000   0.00113  -0.00018   0.00039   2.08171
   A6        2.07472   0.00000   0.00094   0.00005   0.00042   2.07513
   D1       -3.10765  -0.00002  -0.02003   0.00000  -0.02004  -3.12769
   D2       -0.02674   0.00002   0.01577   0.00011   0.01589  -0.01085
   D3        0.03771  -0.00002  -0.02219  -0.00005  -0.02224   0.01547
   D4        3.11862   0.00002   0.01362   0.00007   0.01369   3.13231
        Item               Value     Threshold  Converged?
Maximum Force            0.000175     0.000450     YES
RMS     Force            0.000049     0.000300     YES
Maximum Displacement     0.015905     0.001800     NO
RMS     Displacement     0.005301     0.001200     NO
Predicted change in Energy=-6.656947D-07
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.084595    0.037192    0.050985
     2          8           0       -0.077195    0.152193    1.227216
     3          7           0        1.249237    0.253074   -0.593280
     4          1           0        1.328749    0.154512   -1.578030
     5          1           0        2.047866    0.539360   -0.072430
     6          1           0       -0.719621   -0.262679   -0.622105
---------------------------------------------------------------------
```

```
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.192862   0.000000
    3  N    1.348360   2.254730   0.000000
    4  H    2.053137   3.137847   0.992859   0.000000
    5  H    2.030231   2.520885   0.995516   1.712328   0.000000
    6  H    1.090749   2.001203   2.035493   2.298621   2.933324
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.164622    0.381548    0.000019
     2          8           0       -1.179604   -0.245135    0.000416
     3          7           0        1.073241   -0.153021   -0.002536
     4          1           0        1.888240    0.413911    0.008975
     5          1           0        1.175881   -1.143201    0.005166
     6          1           0       -0.152237    1.472227    0.000168
---------------------------------------------------------------------
Rotational constants (GHZ):     75.6123932     11.6041127     10.0602646
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.0765181967 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.930702570     A.U. after   10 cycles
            Convg  =    0.7939D-08             -V/T =  2.0020
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
---------------------------------------------------------------------
     1        6          -0.000065691   -0.000020684    0.000042487
     2        8          -0.000006067   -0.000000995    0.000000502
     3        7           0.000066068    0.000033030   -0.000042343
     4        1           0.000004969   -0.000009022   -0.000013440
     5        1           0.000010427   -0.000002514    0.000008620
     6        1          -0.000009706    0.000000186    0.000004173
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000066068 RMS     0.000028307

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.000096340 RMS     0.000025857
Search for a local minimum.
Step number  15 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swaping is turned off.
Update second derivatives using D2CorX and points    7    8    9   10   11
                                                    12   13   14   15
DE= -7.89D-07 DEPred=-6.66D-07 R= 1.18D+00
Trust test= 1.18D+00 RLast= 3.66D-02 DXMaxT set to 1.20D+00
The second derivative matrix:
                       R1        R2        R3        R4        R5
         R1          0.82490
         R2          0.10402   0.46550
```

```
          R3           0.00679   0.00626   0.34785
          R4           0.03664  -0.02361   0.00366   0.37159
          R5           0.03690  -0.02259   0.00584   0.00371   0.38988
          A1          -0.02389   0.04167  -0.01708   0.00089   0.00604
          A2           0.03407  -0.03478   0.00573   0.00288  -0.00460
          A3           0.01357   0.01472   0.01072   0.00448   0.01088
          A4          -0.01259   0.04646   0.00259   0.01303   0.01401
          A5          -0.03045   0.02037   0.00544   0.01365   0.02169
          A6           0.01074  -0.04535  -0.00398  -0.01452  -0.01956
          D1          -0.01181  -0.00267   0.00278   0.00352   0.00542
          D2          -0.01113   0.00261   0.00330   0.00444   0.00612
          D3           0.00927   0.01193   0.00054  -0.00034  -0.00181
          D4           0.00995   0.01721   0.00105   0.00058  -0.00111
                         A1        A2        A3        A4        A5
          A1           0.12424
          A2          -0.07110   0.13302
          A3          -0.06144  -0.05197   0.13001
          A4           0.01541  -0.00619  -0.00309   0.11656
          A5          -0.02356   0.00351   0.01902  -0.04389   0.14962
          A6           0.00349   0.00295  -0.01094  -0.04039  -0.05446
          D1           0.00133   0.00453   0.01511  -0.00575   0.00592
          D2           0.00165   0.00350   0.01372  -0.00776   0.00561
          D3           0.00131  -0.00544  -0.01304  -0.00194  -0.00178
          D4           0.00163  -0.00647  -0.01443  -0.00395  -0.00209
                         A6        D1        D2        D3        D4
          A6           0.05109
          D1          -0.00066   0.03325
          D2           0.00088   0.03073   0.02947
          D3           0.00336  -0.02372  -0.02062   0.02294
          D4           0.00490  -0.02623  -0.02188   0.02604   0.03039
     Eigenvalues ---    0.00052   0.00882   0.09816   0.09872   0.15052
     Eigenvalues ---    0.17783   0.22072   0.34924   0.36747   0.38960
     Eigenvalues ---    0.48043   0.858981000.000001000.000001000.00000
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    15   14   13   12   11
 RFO step:  Lambda=-2.13643746D-08.
 DIIS coeffs:      1.68654     -0.16622     -0.89025      0.23118      0.13875
 Iteration  1 RMS(Cart)=  0.00494889 RMS(Int)=  0.00007225
 Iteration  2 RMS(Cart)=  0.00005654 RMS(Int)=  0.00004628
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00004628
 Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                  (DIIS)     (GDIIS)  (Total)
    R1        2.25418   0.00000   0.00000  -0.00002  -0.00001   2.25417
    R2        2.54803   0.00010   0.00009   0.00007   0.00016   2.54819
    R3        2.06122   0.00000  -0.00002   0.00003   0.00001   2.06123
    R4        1.87623   0.00001   0.00002   0.00001   0.00002   1.87625
    R5        1.88125   0.00001   0.00003  -0.00002   0.00002   1.88127
    A1        2.18080   0.00000   0.00001  -0.00002  -0.00001   2.18079
    A2        2.13529  -0.00001  -0.00002   0.00000  -0.00002   2.13527
    A3        1.96710   0.00001   0.00001   0.00002   0.00003   1.96713
    A4        2.12609   0.00000   0.00029  -0.00012   0.00006   2.12614
    A5        2.08171   0.00000   0.00010   0.00003   0.00002   2.08173
    A6        2.07513   0.00000   0.00016   0.00009   0.00015   2.07528
    D1       -3.12769  -0.00001  -0.01876  -0.00007  -0.01884   3.13666
    D2       -0.01085   0.00001   0.01474  -0.00025   0.01449   0.00364
    D3        0.01547  -0.00001  -0.02080  -0.00015  -0.02095  -0.00549
    D4        3.13231   0.00000   0.01270  -0.00033   0.01237  -3.13851
         Item               Value     Threshold  Converged?
 Maximum Force            0.000096     0.000450     YES
 RMS     Force            0.000026     0.000300     YES
 Maximum Displacement     0.014747     0.001800     NO
 RMS     Displacement     0.004948     0.001200     NO
 Predicted change in Energy=-9.777734D-08
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                       Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        0.084345    0.037975    0.050900
      2          8           0       -0.076573    0.149677    1.227562
      3          7           0        1.247231    0.260877   -0.594327
      4          1           0        1.330091    0.149567   -1.577453
      5          1           0        2.048323    0.537852   -0.072208
      6          1           0       -0.719787   -0.262296   -0.622120
 ---------------------------------------------------------------------
                   Distance matrix (angstroms):
                   1          2          3          4          5
    1  C    0.000000
    2  O    1.192856   0.000000
    3  N    1.348446   2.254795   0.000000
    4  H    2.053258   3.137963   0.992871   0.000000
    5  H    2.030330   2.520965   0.995525   1.712421   0.000000
    6  H    1.090756   2.001192   2.035594   2.298759   2.933440
                   6
    6  H    0.000000
 Stoichiometry    CH3NO
 Framework group  C1[X(CH3NO)]
 Deg. of freedom    12
```

```
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.164667    0.381559   -0.000003
     2          8           0        1.179622   -0.245155    0.000155
     3          7           0       -1.073290   -0.153015   -0.000876
     4          1           0       -1.888333    0.413978    0.003193
     5          1           0       -1.175952   -1.143229    0.001713
     6          1           0        0.152342    1.472245    0.000005
---------------------------------------------------------------------
Rotational constants (GHZ):     75.6096034     11.6033975     10.0596132
Standard basis: 6-31G(d) (6D, 7F)
There are    51 symmetry adapted basis functions of A   symmetry.
Integral buffers will be    131072 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
   12 alpha electrons       12 beta electrons
      nuclear repulsion energy        72.0747139681 Hartrees.
NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
One-electron integrals computed using PRISM.
NBasis=    51 RedAO= T  NBF=    51
NBsUse=    51 1.00D-06 NBFU=    51
Initial guess read from the read-write file.
B after Tr=     0.000000    0.000000    0.000000
        Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
Initial guess orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Keep R1 ints in memory in canonical form, NReq=1726457.
SCF Done:  E(RHF) =  -168.930702708     A.U. after   14 cycles
            Convg  =    0.4617D-08             -V/T =  2.0020
Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****
---------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
---------------------------------------------------------------------
     1        6           0.000001236    0.000002959   -0.000002543
     2        8          -0.000001966    0.000001779    0.000001431
     3        7          -0.000007582   -0.000007570    0.000001124
     4        1           0.000004462    0.000006791    0.000002381
     5        1           0.000001371   -0.000001460   -0.000004513
     6        1           0.000002479   -0.000002499    0.000002120
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000007582 RMS     0.000003763

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
Internal  Forces:  Max     0.000006694 RMS     0.000003000
Search for a local minimum.
Step number  16 out of a maximum of   25
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swaping is turned off.
Update second derivatives using D2CorX and points    7    8    9   10   11
                                                    12   13   14   15   16
DE= -1.38D-07 DEPred=-9.78D-08 R= 1.41D+00
Trust test= 1.41D+00 RLast= 3.40D-02 DXMaxT set to 1.20D+00
The second derivative matrix:
                          R1        R2        R3        R4        R5
          R1           0.82301
          R2           0.11495   0.45195
          R3           0.00658   0.00682   0.34796
          R4           0.03744  -0.02668   0.00382   0.37131
          R5           0.03812  -0.02808   0.00601   0.00340   0.38983
          A1          -0.02486   0.04916  -0.01705   0.00146   0.00716
          A2           0.03479  -0.03637   0.00557   0.00229  -0.00557
          A3           0.01539   0.00788   0.01072   0.00388   0.00977
          A4          -0.01671   0.05151   0.00276   0.01461   0.01646
          A5          -0.03725   0.02669   0.00602   0.01633   0.02570
          A6           0.01683  -0.05013  -0.00437  -0.01669  -0.02298
          D1          -0.01270  -0.00147   0.00271   0.00370   0.00569
          D2          -0.01203   0.00309   0.00335   0.00466   0.00645
          D3           0.00982   0.01153   0.00042  -0.00055  -0.00206
          D4           0.01048   0.01609   0.00105   0.00041  -0.00130
```

```
                          A1        A2        A3        A4        A5
          A1           0.12459
          A2          -0.07139   0.13302
          A3          -0.06059  -0.05188   0.12814
          A4           0.01358  -0.00531  -0.00154   0.11396
          A5          -0.02630   0.00412   0.02120  -0.04620   0.14996
          A6           0.00600   0.00202  -0.01282  -0.03777  -0.05382
          D1           0.00067   0.00480   0.01562  -0.00639   0.00514
          D2           0.00107   0.00385   0.01403  -0.00844   0.00508
          D3           0.00168  -0.00542  -0.01324  -0.00193  -0.00225
          D4           0.00208  -0.00638  -0.01483  -0.00398  -0.00231
                          A6        D1        D2        D3        D4
          A6           0.04960
          D1           0.00000   0.03320
          D2           0.00160   0.03068   0.02923
          D3           0.00351  -0.02365  -0.02062   0.02311
          D4           0.00511  -0.02618  -0.02207   0.02614   0.03025
    Eigenvalues ---    0.00044   0.00798   0.08236   0.09827   0.14946
    Eigenvalues ---    0.17741   0.22280   0.34920   0.36716   0.38934
    Eigenvalues ---    0.47419   0.861851000.000001000.000001000.00000
En-DIIS/RFO-DIIS IScMMF=        0 using points:    16   15   14   13   12
RFO step:  Lambda= 0.00000000D+00.
DIIS coeffs:      0.62960      0.60398     -0.28975      0.04385      0.01231
Iteration  1 RMS(Cart)=  0.00113173 RMS(Int)=  0.00001295
Iteration  2 RMS(Cart)=  0.00000290 RMS(Int)=  0.00001263
Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00001263
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                  (DIIS)     (GDIIS)  (Total)
   R1        2.25417   0.00000   0.00000   0.00001   0.00001   2.25418
   R2        2.54819   0.00000  -0.00004   0.00003  -0.00001   2.54818
   R3        2.06123   0.00000  -0.00001   0.00000  -0.00001   2.06122
   R4        1.87625   0.00000   0.00000   0.00000  -0.00001   1.87625
   R5        1.88127   0.00000   0.00000  -0.00001  -0.00001   1.88126
   A1        2.18079   0.00000  -0.00001   0.00003   0.00001   2.18080
   A2        2.13527   0.00000   0.00001  -0.00001  -0.00001   2.13526
   A3        1.96713   0.00000   0.00001  -0.00001  -0.00001   1.96712
   A4        2.12614   0.00000   0.00001   0.00002   0.00006   2.12620
   A5        2.08173   0.00000  -0.00002   0.00002   0.00002   2.08176
   A6        2.07528  -0.00001  -0.00004  -0.00004  -0.00005   2.07523
   D1        3.13666   0.00000   0.00423   0.00013   0.00436   3.14102
   D2        0.00364   0.00000  -0.00318   0.00006  -0.00313   0.00051
   D3       -0.00549   0.00000   0.00472   0.00012   0.00484  -0.00065
   D4       -3.13851   0.00000  -0.00269   0.00004  -0.00265  -3.14116
        Item               Value     Threshold  Converged?
Maximum Force            0.000007     0.000450     YES
RMS     Force            0.000003     0.000300     YES
Maximum Displacement     0.003312     0.001800     NO
RMS     Displacement     0.001132     0.001200     YES
Predicted change in Energy=-1.809809D-08
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.084388    0.037797    0.050930
     2          8           0       -0.076747    0.150289    1.227491
     3          7           0        1.247680    0.259125   -0.594097
     4          1           0        1.329811    0.150748   -1.577609
     5          1           0        2.048249    0.538132   -0.072267
     6          1           0       -0.719750   -0.262440   -0.622093
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.192860   0.000000
    3  N    1.348441   2.254803   0.000000
    4  H    2.053283   3.137991   0.992867   0.000000
    5  H    2.030335   2.520993   0.995521   1.712388   0.000000
    6  H    1.090752   2.001189   2.035582   2.298790   2.933435
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.164666    0.381555    0.000005
     2          8           0        1.179629   -0.245154    0.000015
     3          7           0       -1.073290   -0.153009   -0.000112
     4          1           0       -1.888362    0.413951    0.000369
     5          1           0       -1.175977   -1.143220    0.000245
```

```
     6          1           0        0.152340    1.472237    0.000017
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     75.6114324     11.6032817     10.0595498
 Standard basis: 6-31G(d) (6D, 7F)
 There are    51 symmetry adapted basis functions of A   symmetry.
 Integral buffers will be    131072 words long.
 Raffenetti 1 integral format.
 Two-electron integral symmetry is turned on.
    51 basis functions,    96 primitive gaussians,    51 cartesian basis functions
    12 alpha electrons       12 beta electrons
       nuclear repulsion energy        72.0746475812 Hartrees.
 NAtoms=    6 NActive=    6 NUniq=    6 SFac= 7.50D-01 NAtFMM=   80 NAOKFM=F Big=F
 One-electron integrals computed using PRISM.
 NBasis=    51 RedAO= T  NBF=    51
 NBsUse=    51 1.00D-06 NBFU=    51
 Initial guess read from the read-write file.
 B after Tr=     0.000000    0.000000    0.000000
         Rot=    1.000000    0.000000    0.000000    0.000000 Ang=   0.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A)
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 ints in memory in canonical form, NReq=1726457.
 SCF Done:  E(RHF) =  -168.930702726     A.U. after    9 cycles
             Convg  =    0.6928D-08             -V/T =  2.0020
 Calling FoFJK, ICntrl=      2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6          -0.000003846    0.000001706    0.000002700
      2        8           0.000003089   -0.000001385   -0.000006592
      3        7           0.000000363   -0.000001313    0.000002911
      4        1          -0.000001539   -0.000000850   -0.000001006
      5        1           0.000002210    0.000001903    0.000001527
      6        1          -0.000000277   -0.000000060    0.000000462
 -------------------------------------------------------------------
 Cartesian Forces:  Max     0.000006592 RMS     0.000002421

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 Internal  Forces:  Max     0.000007050 RMS     0.000002413
 Search for a local minimum.
 Step number  17 out of a maximum of   25
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swaping is turned off.
 Update second derivatives using D2CorX and points    7    8    9   10   11
                                                     12   13   14   15   16
                                                     17
 DE= -1.82D-08 DEPred=-1.81D-08 R= 1.01D+00
 Trust test= 1.01D+00 RLast= 7.70D-03 DXMaxT set to 1.20D+00
 The second derivative matrix:
                        R1        R2        R3        R4        R5
          R1           0.82661
          R2           0.12049   0.44622
          R3           0.00514   0.00792   0.34821
          R4           0.03579  -0.02750   0.00435   0.37197
          R5           0.03584  -0.03051   0.00686   0.00457   0.39191
          A1          -0.02378   0.05343  -0.01754   0.00102   0.00681
          A2           0.03458  -0.03746   0.00562   0.00203  -0.00593
          A3           0.01572   0.00365   0.01116   0.00415   0.00967
          A4          -0.01742   0.05322   0.00237   0.01493   0.01667
          A5          -0.04356   0.03079   0.00656   0.01879   0.02910
          A6           0.01906  -0.05223  -0.00423  -0.01762  -0.02405
          D1          -0.01189  -0.00135   0.00242   0.00332   0.00497
          D2          -0.01121   0.00323   0.00304   0.00426   0.00578
          D3           0.01158   0.01040   0.00022  -0.00107  -0.00298
          D4           0.01226   0.01499   0.00084  -0.00013  -0.00218
                         A1        A2        A3        A4        A5
          A1           0.12544
          A2          -0.07192   0.13300
          A3          -0.06033  -0.05140   0.12656
          A4           0.01288  -0.00466  -0.00149   0.11273
          A5          -0.02907   0.00532   0.02253  -0.04902   0.14920
          A6           0.00692   0.00129  -0.01275  -0.03666  -0.05249
          D1           0.00072   0.00482   0.01543  -0.00624   0.00436
          D2           0.00127   0.00391   0.01383  -0.00822   0.00438
          D3           0.00247  -0.00558  -0.01399  -0.00152  -0.00276
          D4           0.00301  -0.00649  -0.01559  -0.00350  -0.00275
                         A6        D1        D2        D3        D4
```

```
          A6           0.04947
          D1          -0.00019   0.03357
          D2           0.00152   0.03104   0.02952
          D3           0.00317  -0.02336  -0.02029   0.02328
          D4           0.00488  -0.02589  -0.02180   0.02636   0.03045
    Eigenvalues ---    0.00037   0.00943   0.07329   0.09819   0.14867
    Eigenvalues ---    0.17708   0.22491   0.34917   0.36831   0.39175
    Eigenvalues ---    0.47221   0.867171000.000001000.000001000.00000
En-DIIS/RFO-DIIS IScMMF=        0 using points:    17   16   15   14   13
RFO step:  Lambda= 0.00000000D+00.
DIIS coeffs:      0.71575      0.25055      0.10517     -0.13229      0.06082
Iteration  1 RMS(Cart)=  0.00004243 RMS(Int)=  0.00002550
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00002550
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                  (DIIS)     (GDIIS)  (Total)
   R1        2.25418  -0.00001  -0.00001   0.00000  -0.00001   2.25417
   R2        2.54818   0.00000   0.00002   0.00000   0.00002   2.54821
   R3        2.06122   0.00000   0.00000   0.00000   0.00000   2.06122
   R4        1.87625   0.00000   0.00001   0.00000   0.00001   1.87625
   R5        1.88126   0.00000   0.00001   0.00001   0.00001   1.88127
   A1        2.18080   0.00000  -0.00002   0.00000  -0.00001   2.18079
   A2        2.13526   0.00000   0.00000   0.00000   0.00000   2.13527
   A3        1.96712   0.00000   0.00001   0.00000   0.00001   1.96713
   A4        2.12620   0.00000  -0.00006  -0.00001  -0.00001   2.12619
   A5        2.08176   0.00000  -0.00007   0.00001   0.00000   2.08175
   A6        2.07523   0.00000  -0.00004   0.00000   0.00002   2.07524
   D1        3.14102   0.00000  -0.00018   0.00001  -0.00017   3.14085
   D2        0.00051   0.00000   0.00008  -0.00002   0.00006   0.00057
   D3       -0.00065   0.00000  -0.00019   0.00002  -0.00017  -0.00082
   D4       -3.14116   0.00000   0.00006  -0.00001   0.00006  -3.14110
        Item               Value     Threshold  Converged?
Maximum Force            0.000007     0.000450     YES
RMS     Force            0.000002     0.000300     YES
Maximum Displacement     0.000103     0.001800     YES
RMS     Displacement     0.000042     0.001200     YES
Predicted change in Energy=-4.242055D-11
Optimization completed.
   -- Stationary point found.
                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.1929         -DE/DX =    0.0                 !
! R2    R(1,3)                  1.3484         -DE/DX =    0.0                 !
! R3    R(1,6)                  1.0908         -DE/DX =    0.0                 !
! R4    R(3,4)                  0.9929         -DE/DX =    0.0                 !
! R5    R(3,5)                  0.9955         -DE/DX =    0.0                 !
! A1    A(2,1,3)              124.9507         -DE/DX =    0.0                 !
! A2    A(2,1,6)              122.3415         -DE/DX =    0.0                 !
! A3    A(3,1,6)              112.7078         -DE/DX =    0.0                 !
! A4    A(1,3,4)              121.8224         -DE/DX =    0.0                 !
! A5    A(1,3,5)              119.2758         -DE/DX =    0.0                 !
! A6    A(4,3,5)              118.9017         -DE/DX =    0.0                 !
! D1    D(2,1,3,4)            179.9672         -DE/DX =    0.0                 !
! D2    D(2,1,3,5)              0.0293         -DE/DX =    0.0                 !
! D3    D(6,1,3,4)             -0.0372         -DE/DX =    0.0                 !
! D4    D(6,1,3,5)           -179.9751         -DE/DX =    0.0                 !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.084388    0.037797    0.050930
     2          8           0       -0.076747    0.150289    1.227491
     3          7           0        1.247680    0.259125   -0.594097
     4          1           0        1.329811    0.150748   -1.577609
     5          1           0        2.048249    0.538132   -0.072267
     6          1           0       -0.719750   -0.262440   -0.622093
---------------------------------------------------------------------
                  Distance matrix (angstroms):
                  1          2          3          4          5
    1  C    0.000000
    2  O    1.192860   0.000000
    3  N    1.348441   2.254803   0.000000
    4  H    2.053283   3.137991   0.992867   0.000000
    5  H    2.030335   2.520993   0.995521   1.712388   0.000000
    6  H    1.090752   2.001189   2.035582   2.298790   2.933435
                  6
    6  H    0.000000
Stoichiometry    CH3NO
Framework group  C1[X(CH3NO)]
Deg. of freedom    12
Full point group                 C1      NOp   1
Largest Abelian subgroup         C1      NOp   1
```

```
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type             X           Y           Z
---------------------------------------------------------------------
     1          6           0        0.164666    0.381555    0.000005
     2          8           0        1.179629   -0.245154    0.000015
     3          7           0       -1.073290   -0.153009   -0.000112
     4          1           0       -1.888362    0.413951    0.000369
     5          1           0       -1.175977   -1.143220    0.000245
     6          1           0        0.152340    1.472237    0.000017
---------------------------------------------------------------------
Rotational constants (GHZ):     75.6114324     11.6032817     10.0595498

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

          Population analysis using the SCF density.

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

Orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A)
The electronic state is 1-A.
Alpha  occ. eigenvalues --  -20.53007 -15.59117 -11.35051  -1.39318  -1.22011
Alpha  occ. eigenvalues --   -0.85018  -0.75335  -0.67373  -0.60708  -0.57158
Alpha  occ. eigenvalues --   -0.42856  -0.41490
Alpha virt. eigenvalues --    0.21169   0.22134   0.25869   0.31745   0.42816
Alpha virt. eigenvalues --    0.54629   0.75024   0.75708   0.86322   0.92804
Alpha virt. eigenvalues --    0.96551   0.98913   1.07214   1.12011   1.16985
Alpha virt. eigenvalues --    1.19860   1.30835   1.33534   1.46142   1.57332
Alpha virt. eigenvalues --    1.64175   1.74795   1.75790   1.98165   2.06493
Alpha virt. eigenvalues --    2.15733   2.20319   2.36719   2.47684   2.63463
Alpha virt. eigenvalues --    2.63872   2.85674   2.99712   3.04805   3.31234
Alpha virt. eigenvalues --    3.41750   4.16833   4.30940   4.60101
         Condensed to atoms (all electrons):
              1          2          3          4          5          6
    1  C    4.225739   0.612851   0.263635  -0.013646  -0.009397   0.412476
    2  O    0.612851   8.077572  -0.092347   0.002376   0.006251  -0.052041
    3  N    0.263635  -0.092347   7.197288   0.316620   0.307622  -0.108559
    4  H   -0.013646   0.002376   0.316620   0.314276  -0.012338   0.003798
    5  H   -0.009397   0.006251   0.307622  -0.012338   0.304746   0.004753
    6  H    0.412476  -0.052041  -0.108559   0.003798   0.004753   0.596267
Mulliken atomic charges:
              1
    1  C    0.508341
    2  O   -0.554663
    3  N   -0.884260
    4  H    0.388913
    5  H    0.398363
    6  H    0.143306
Sum of Mulliken atomic charges =   0.00000
Mulliken charges with hydrogens summed into heavy atoms:
              1
    1  C    0.651647
    2  O   -0.554663
    3  N   -0.096984
Sum of Mulliken charges with hydrogens summed into heavy atoms =   0.00000
Electronic spatial extent (au):  =            143.4380
Charge=              0.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=             -3.9411    Y=              1.1329    Z=              0.0016  Tot=              4.1006
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=            -17.9625   YY=            -14.7904   ZZ=            -18.5077
  XY=              1.1987   XZ=             -0.0028   YZ=             -0.0004
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=             -0.8756   YY=              2.2965   ZZ=             -1.4208
  XY=              1.1987   XZ=             -0.0028   YZ=             -0.0004
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=            -12.6701  YYY=             -2.0382  ZZZ=              0.0015  XYY=             -2.8702
 XXY=              1.1490  XXZ=              0.0046  XZZ=              1.5311  YZZ=             -0.0666
 YYZ=              0.0012  XYZ=              0.0003
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=           -104.0653 YYYY=            -30.3872 ZZZZ=            -15.6663 XXXY=             -2.4935
XXXZ=             -0.0089 YYYX=              3.1962 YYYZ=             -0.0010 ZZZX=             -0.0023
ZZZY=             -0.0003 XXYY=            -21.5219 XXZZ=            -23.5949 YYZZ=             -8.6628
XXYZ=              0.0001 YYXZ=             -0.0017 ZZXY=             -0.2832
N-N= 7.207464758118D+01 E-N=-5.418272847292D+02  KE= 1.685854613484D+02
B after Tr=     0.985181    0.068790    0.338368
        Rot=   -0.260706    0.338763   -0.587370    0.687218 Ang= 210.22 deg.
Final structure in terms of initial Z-matrix:
C
O,1,B1
N,1,B2,2,A1
H,3,B3,1,A2,2,D1,0
```

```
H,3,B4,1,A3,2,D2,0
H,1,B5,2,A4,3,D3,0
     Variables:
B1=1.19286035
B2=1.3484412
B3=0.99286732
B4=0.99552067
B5=1.09075217
A1=124.95067179
A2=121.82244459
A3=119.27579503
A4=122.34153253
D1=179.96720531
D2=0.0292918
D3=-179.99521742
1\1\GINC-BUCHNER\FOpt\RHF\6-31G(d)\C1H3N1O1\WEBMODEMO\12-Mar-2012\0\\#
N HF/6-31G(d) OPT(NewEstmFC) Geom=Connectivity\\CH3ON\\0,1\C,0.0843883
61,0.0377971172,0.050929685\O,-0.0767474704,0.1502887078,1.2274910711\
N,1.247680335,0.2591246906,-0.594097108\H,1.3298108539,0.1507484355,-1
.5776085127\H,2.0482489354,0.5381320359,-0.0722674262\H,-0.7197502177,
-0.2624396454,-0.6220928409\\Version=AM64L-G09RevA.02\State=1-A\HF=-16
8.9307027\RMSD=6.928e-09\RMSF=2.421e-06\Dipole=0.6271622,-0.0312741,-1
.4860983\Quadrupole=1.450572,-0.8155711,-0.635001,0.7726899,0.8698195,
0.2858895\PG=C01 [X(C1H3N1O1)]\\@
```

```
Job cpu time:  0 days  0 hours  0 minutes 36.2 seconds.
File lengths (MBytes):  RWF=      5 Int=      0 D2E=      0 Chk=      1 Scr=      1
Normal termination of Gaussian 09 at Mon Mar 12 22:29:13 2012.
```