Entering Gaussian System, Link 0=g16
Initial command:
/share/apps/compute/gaussian/16.B.01/g16/l1.exe
"/oasis/scratch/comet/gridchem/temp_project/38158479/Gau-23423.inp"
-scrdir="/oasis/scratch/comet/gridchem/temp_project/38158479/"
Entering Link 1 = /share/apps/compute/gaussian/16.B.01/g16/l1.exe PID= 23425.

```
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 16, Revision B.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone,
G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich,
J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian,
J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young,
F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone,
T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega,
G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda,
J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai,
T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta,
F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin,
V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar,
J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi,
J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas,
J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

****************************************
Gaussian 16:  ES64L-G16RevB.01 20-Dec-2017
               31-Jan-2021
****************************************
%mem=5000MW
%nprocshared=16
Will use up to   16 processors via shared memory.
----------------------------------------------------------------------
# opt=(calcfc,maxcycle=500) freq=noraman b3lyp/3-21g* symm=(follow,pg=
d5h)
----------------------------------------------------------------------
1/6=500,10=4,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,19=2314885530821080388,40=1/2;
3/5=5,7=1,11=2,25=1,30=1,71=2,74=-5,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/10=1,18=20,25=1/1,2,3,16;
1/6=500,10=4,18=20,19=15,26=3/3(2);
2/9=110,15=5,19=2314885530821080388/2;
99//99;
```

```
2/9=110,15=5,19=2314885530821080388/2;
3/5=5,7=1,11=2,25=1,30=1,71=1,74=-5/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/6=500,18=20,19=15,26=3/3(-5);
2/9=110,15=5,19=2314885530821080388/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
---------------------
<Calculation as sent>
---------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                     0.        1.22497  -1.88346
C                    -1.16502   0.37854  -1.88346
C                    -0.72002  -0.99102  -1.88346
C                     0.72002  -0.99102  -1.88346
C                     1.16502   0.37854  -1.88346
H                    -2.18981   0.71151  -1.92642
H                    -1.35337  -1.86276  -1.92642
H                     1.35337  -1.86276  -1.92642
H                     2.18981   0.71151  -1.92642
H                     0.        2.3025   -1.92642
C                     0.        1.22497   1.88346
C                    -1.16502   0.37854   1.88346
C                    -0.72002  -0.99102   1.88346
C                     0.72002  -0.99102   1.88346
C                     1.16502   0.37854   1.88346
H                     0.        2.3025    1.92642
H                    -2.18981   0.71151   1.92642
H                    -1.35337  -1.86276   1.92642
H                     1.35337  -1.86276   1.92642
H                     2.18981   0.71151   1.92642
Ru                    0.        0.        0.


GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.44           calculate D2E/DX2 analytically  !
! R2    R(1,5)                  1.44           calculate D2E/DX2 analytically  !
! R3    R(1,10)                 1.0784         calculate D2E/DX2 analytically  !
! R4    R(1,21)                 2.2468         calculate D2E/DX2 analytically  !
```

```
! R5    R(2,3)              1.44          calculate D2E/DX2 analytically  !
! R6    R(2,6)              1.0784        calculate D2E/DX2 analytically  !
! R7    R(2,21)             2.2468        calculate D2E/DX2 analytically  !
! R8    R(3,4)              1.44          calculate D2E/DX2 analytically  !
! R9    R(3,7)              1.0784        calculate D2E/DX2 analytically  !
! R10   R(3,21)             2.2468        calculate D2E/DX2 analytically  !
! R11   R(4,5)              1.44          calculate D2E/DX2 analytically  !
! R12   R(4,8)              1.0784        calculate D2E/DX2 analytically  !
! R13   R(4,21)             2.2468        calculate D2E/DX2 analytically  !
! R14   R(5,9)              1.0784        calculate D2E/DX2 analytically  !
! R15   R(5,21)             2.2468        calculate D2E/DX2 analytically  !
! R16   R(11,12)            1.44          calculate D2E/DX2 analytically  !
! R17   R(11,15)            1.44          calculate D2E/DX2 analytically  !
! R18   R(11,16)            1.0784        calculate D2E/DX2 analytically  !
! R19   R(11,21)            2.2468        calculate D2E/DX2 analytically  !
! R20   R(12,13)            1.44          calculate D2E/DX2 analytically  !
! R21   R(12,17)            1.0784        calculate D2E/DX2 analytically  !
! R22   R(12,21)            2.2468        calculate D2E/DX2 analytically  !
! R23   R(13,14)            1.44          calculate D2E/DX2 analytically  !
! R24   R(13,18)            1.0784        calculate D2E/DX2 analytically  !
! R25   R(13,21)            2.2468        calculate D2E/DX2 analytically  !
! R26   R(14,15)            1.44          calculate D2E/DX2 analytically  !
! R27   R(14,19)            1.0784        calculate D2E/DX2 analytically  !
! R28   R(14,21)            2.2468        calculate D2E/DX2 analytically  !
! R29   R(15,20)            1.0784        calculate D2E/DX2 analytically  !
! R30   R(15,21)            2.2468        calculate D2E/DX2 analytically  !
! A1    A(2,1,5)            108.0         calculate D2E/DX2 analytically  !
! A2    A(2,1,10)           125.967       calculate D2E/DX2 analytically  !
! A3    A(5,1,10)           125.967       calculate D2E/DX2 analytically  !
! A4    A(10,1,21)          125.3225      calculate D2E/DX2 analytically  !
! A5    A(1,2,3)            108.0         calculate D2E/DX2 analytically  !
! A6    A(1,2,6)            125.967       calculate D2E/DX2 analytically  !
! A7    A(3,2,6)            125.967       calculate D2E/DX2 analytically  !
! A8    A(6,2,21)           125.3225      calculate D2E/DX2 analytically  !
! A9    A(2,3,4)            108.0         calculate D2E/DX2 analytically  !
! A10   A(2,3,7)            125.967       calculate D2E/DX2 analytically  !
! A11   A(4,3,7)            125.967       calculate D2E/DX2 analytically  !
! A12   A(7,3,21)           125.3225      calculate D2E/DX2 analytically  !
! A13   A(3,4,5)            108.0         calculate D2E/DX2 analytically  !
! A14   A(3,4,8)            125.967       calculate D2E/DX2 analytically  !
! A15   A(5,4,8)            125.967       calculate D2E/DX2 analytically  !
! A16   A(8,4,21)           125.3225      calculate D2E/DX2 analytically  !
! A17   A(1,5,4)            108.0         calculate D2E/DX2 analytically  !
! A18   A(1,5,9)            125.967       calculate D2E/DX2 analytically  !
! A19   A(4,5,9)            125.967       calculate D2E/DX2 analytically  !
! A20   A(9,5,21)           125.3225      calculate D2E/DX2 analytically  !
! A21   A(12,11,15)         108.0         calculate D2E/DX2 analytically  !
! A22   A(12,11,16)         125.967       calculate D2E/DX2 analytically  !
! A23   A(15,11,16)         125.967       calculate D2E/DX2 analytically  !
! A24   A(16,11,21)         125.3225      calculate D2E/DX2 analytically  !
```

```
! A25   A(11,12,13)          108.0           calculate D2E/DX2 analytically  !
! A26   A(11,12,17)          125.967         calculate D2E/DX2 analytically  !
! A27   A(13,12,17)          125.967         calculate D2E/DX2 analytically  !
! A28   A(17,12,21)          125.3225        calculate D2E/DX2 analytically  !
! A29   A(12,13,14)          108.0           calculate D2E/DX2 analytically  !
! A30   A(12,13,18)          125.967         calculate D2E/DX2 analytically  !
! A31   A(14,13,18)          125.967         calculate D2E/DX2 analytically  !
! A32   A(18,13,21)          125.3225        calculate D2E/DX2 analytically  !
! A33   A(13,14,15)          108.0           calculate D2E/DX2 analytically  !
! A34   A(13,14,19)          125.967         calculate D2E/DX2 analytically  !
! A35   A(15,14,19)          125.967         calculate D2E/DX2 analytically  !
! A36   A(19,14,21)          125.3225        calculate D2E/DX2 analytically  !
! A37   A(11,15,14)          108.0           calculate D2E/DX2 analytically  !
! A38   A(11,15,20)          125.967         calculate D2E/DX2 analytically  !
! A39   A(14,15,20)          125.967         calculate D2E/DX2 analytically  !
! A40   A(20,15,21)          125.3225        calculate D2E/DX2 analytically  !
! A41   A(1,21,3)             62.4674        calculate D2E/DX2 analytically  !
! A42   A(1,21,4)             62.4674        calculate D2E/DX2 analytically  !
! A43   A(1,21,11)           113.9213        calculate D2E/DX2 analytically  !
! A44   A(1,21,12)           127.6534        calculate D2E/DX2 analytically  !
! A45   A(1,21,13)           160.601         calculate D2E/DX2 analytically  !
! A46   A(1,21,14)           160.601         calculate D2E/DX2 analytically  !
! A47   A(1,21,15)           127.6534        calculate D2E/DX2 analytically  !
! A48   A(2,21,4)             62.4674        calculate D2E/DX2 analytically  !
! A49   A(2,21,5)             62.4674        calculate D2E/DX2 analytically  !
! A50   A(2,21,11)           127.6534        calculate D2E/DX2 analytically  !
! A51   A(2,21,12)           113.9213        calculate D2E/DX2 analytically  !
! A52   A(2,21,13)           127.6534        calculate D2E/DX2 analytically  !
! A53   A(2,21,14)           160.601         calculate D2E/DX2 analytically  !
! A54   A(2,21,15)           160.601         calculate D2E/DX2 analytically  !
! A55   A(3,21,5)             62.4674        calculate D2E/DX2 analytically  !
! A56   A(3,21,11)           160.601         calculate D2E/DX2 analytically  !
! A57   A(3,21,12)           127.6534        calculate D2E/DX2 analytically  !
! A58   A(3,21,13)           113.9213        calculate D2E/DX2 analytically  !
! A59   A(3,21,14)           127.6534        calculate D2E/DX2 analytically  !
! A60   A(3,21,15)           160.601         calculate D2E/DX2 analytically  !
! A61   A(4,21,11)           160.601         calculate D2E/DX2 analytically  !
! A62   A(4,21,12)           160.601         calculate D2E/DX2 analytically  !
! A63   A(4,21,13)           127.6534        calculate D2E/DX2 analytically  !
! A64   A(4,21,14)           113.9213        calculate D2E/DX2 analytically  !
! A65   A(4,21,15)           127.6534        calculate D2E/DX2 analytically  !
! A66   A(5,21,11)           127.6534        calculate D2E/DX2 analytically  !
! A67   A(5,21,12)           160.601         calculate D2E/DX2 analytically  !
! A68   A(5,21,13)           160.601         calculate D2E/DX2 analytically  !
! A69   A(5,21,14)           127.6534        calculate D2E/DX2 analytically  !
! A70   A(5,21,15)           113.9213        calculate D2E/DX2 analytically  !
! A71   A(11,21,13)           62.4674        calculate D2E/DX2 analytically  !
! A72   A(11,21,14)           62.4674        calculate D2E/DX2 analytically  !
! A73   A(12,21,14)           62.4674        calculate D2E/DX2 analytically  !
! A74   A(12,21,15)           62.4674        calculate D2E/DX2 analytically  !
```

```
! A75   A(13,21,15)          62.4674        calculate D2E/DX2 analytically  !
! D1    D(5,1,2,3)            0.0          calculate D2E/DX2 analytically  !
! D2    D(5,1,2,6)         -177.1787       calculate D2E/DX2 analytically  !
! D3    D(10,1,2,3)         177.1787       calculate D2E/DX2 analytically  !
! D4    D(10,1,2,6)           0.0          calculate D2E/DX2 analytically  !
! D5    D(2,1,5,4)            0.0          calculate D2E/DX2 analytically  !
! D6    D(2,1,5,9)          177.1787       calculate D2E/DX2 analytically  !
! D7    D(10,1,5,4)        -177.1787       calculate D2E/DX2 analytically  !
! D8    D(10,1,5,9)           0.0          calculate D2E/DX2 analytically  !
! D9    D(10,1,21,3)        158.8139       calculate D2E/DX2 analytically  !
! D10   D(10,1,21,4)       -158.8139       calculate D2E/DX2 analytically  !
! D11   D(10,1,21,11)          0.0          calculate D2E/DX2 analytically  !
! D12   D(10,1,21,12)         40.9151       calculate D2E/DX2 analytically  !
! D13   D(10,1,21,13)         74.7635       calculate D2E/DX2 analytically  !
! D14   D(10,1,21,14)        -74.7635       calculate D2E/DX2 analytically  !
! D15   D(10,1,21,15)        -40.9151       calculate D2E/DX2 analytically  !
! D16   D(1,2,3,4)             0.0          calculate D2E/DX2 analytically  !
! D17   D(1,2,3,7)          -177.1787       calculate D2E/DX2 analytically  !
! D18   D(6,2,3,4)           177.1787       calculate D2E/DX2 analytically  !
! D19   D(6,2,3,7)             0.0          calculate D2E/DX2 analytically  !
! D20   D(6,2,21,4)          158.8139       calculate D2E/DX2 analytically  !
! D21   D(6,2,21,5)         -158.8139       calculate D2E/DX2 analytically  !
! D22   D(6,2,21,11)         -40.9151       calculate D2E/DX2 analytically  !
! D23   D(6,2,21,12)           0.0          calculate D2E/DX2 analytically  !
! D24   D(6,2,21,13)          40.9151       calculate D2E/DX2 analytically  !
! D25   D(6,2,21,14)          74.7635       calculate D2E/DX2 analytically  !
! D26   D(6,2,21,15)         -74.7635       calculate D2E/DX2 analytically  !
! D27   D(2,3,4,5)             0.0          calculate D2E/DX2 analytically  !
! D28   D(2,3,4,8)          -177.1787       calculate D2E/DX2 analytically  !
! D29   D(7,3,4,5)           177.1787       calculate D2E/DX2 analytically  !
! D30   D(7,3,4,8)             0.0          calculate D2E/DX2 analytically  !
! D31   D(7,3,21,1)         -158.8139       calculate D2E/DX2 analytically  !
! D32   D(7,3,21,5)          158.8139       calculate D2E/DX2 analytically  !
! D33   D(7,3,21,11)         -74.7635       calculate D2E/DX2 analytically  !
! D34   D(7,3,21,12)         -40.9151       calculate D2E/DX2 analytically  !
! D35   D(7,3,21,13)           0.0          calculate D2E/DX2 analytically  !
! D36   D(7,3,21,14)          40.9151       calculate D2E/DX2 analytically  !
! D37   D(7,3,21,15)          74.7635       calculate D2E/DX2 analytically  !
! D38   D(3,4,5,1)             0.0          calculate D2E/DX2 analytically  !
! D39   D(3,4,5,9)          -177.1787       calculate D2E/DX2 analytically  !
! D40   D(8,4,5,1)           177.1787       calculate D2E/DX2 analytically  !
! D41   D(8,4,5,9)             0.0          calculate D2E/DX2 analytically  !
! D42   D(8,4,21,1)          158.8139       calculate D2E/DX2 analytically  !
! D43   D(8,4,21,2)         -158.8139       calculate D2E/DX2 analytically  !
! D44   D(8,4,21,11)          74.7635       calculate D2E/DX2 analytically  !
! D45   D(8,4,21,12)         -74.7635       calculate D2E/DX2 analytically  !
! D46   D(8,4,21,13)         -40.9151       calculate D2E/DX2 analytically  !
! D47   D(8,4,21,14)           0.0          calculate D2E/DX2 analytically  !
! D48   D(8,4,21,15)          40.9151       calculate D2E/DX2 analytically  !
! D49   D(9,5,21,2)          158.8139       calculate D2E/DX2 analytically  !
```

```
! D50   D(9,5,21,3)          -158.8139         calculate D2E/DX2 analytically  !
! D51   D(9,5,21,11)           40.9151         calculate D2E/DX2 analytically  !
! D52   D(9,5,21,12)           74.7635         calculate D2E/DX2 analytically  !
! D53   D(9,5,21,13)          -74.7635         calculate D2E/DX2 analytically  !
! D54   D(9,5,21,14)          -40.9151         calculate D2E/DX2 analytically  !
! D55   D(9,5,21,15)            0.0            calculate D2E/DX2 analytically  !
! D56   D(15,11,12,13)          0.0            calculate D2E/DX2 analytically  !
! D57   D(15,11,12,17)        177.1787         calculate D2E/DX2 analytically  !
! D58   D(16,11,12,13)       -177.1787         calculate D2E/DX2 analytically  !
! D59   D(16,11,12,17)          0.0            calculate D2E/DX2 analytically  !
! D60   D(12,11,15,14)          0.0            calculate D2E/DX2 analytically  !
! D61   D(12,11,15,20)       -177.1787         calculate D2E/DX2 analytically  !
! D62   D(16,11,15,14)        177.1787         calculate D2E/DX2 analytically  !
! D63   D(16,11,15,20)          0.0            calculate D2E/DX2 analytically  !
! D64   D(16,11,21,1)           0.0            calculate D2E/DX2 analytically  !
! D65   D(16,11,21,2)         -40.9151         calculate D2E/DX2 analytically  !
! D66   D(16,11,21,3)         -74.7635         calculate D2E/DX2 analytically  !
! D67   D(16,11,21,4)          74.7635         calculate D2E/DX2 analytically  !
! D68   D(16,11,21,5)          40.9151         calculate D2E/DX2 analytically  !
! D69   D(16,11,21,13)       -158.8139         calculate D2E/DX2 analytically  !
! D70   D(16,11,21,14)        158.8139         calculate D2E/DX2 analytically  !
! D71   D(11,12,13,14)          0.0            calculate D2E/DX2 analytically  !
! D72   D(11,12,13,18)        177.1787         calculate D2E/DX2 analytically  !
! D73   D(17,12,13,14)       -177.1787         calculate D2E/DX2 analytically  !
! D74   D(17,12,13,18)          0.0            calculate D2E/DX2 analytically  !
! D75   D(17,12,21,1)          40.9151         calculate D2E/DX2 analytically  !
! D76   D(17,12,21,2)           0.0            calculate D2E/DX2 analytically  !
! D77   D(17,12,21,3)         -40.9151         calculate D2E/DX2 analytically  !
! D78   D(17,12,21,4)         -74.7635         calculate D2E/DX2 analytically  !
! D79   D(17,12,21,5)          74.7635         calculate D2E/DX2 analytically  !
! D80   D(17,12,21,14)       -158.8139         calculate D2E/DX2 analytically  !
! D81   D(17,12,21,15)        158.8139         calculate D2E/DX2 analytically  !
! D82   D(12,13,14,15)          0.0            calculate D2E/DX2 analytically  !
! D83   D(12,13,14,19)        177.1787         calculate D2E/DX2 analytically  !
! D84   D(18,13,14,15)       -177.1787         calculate D2E/DX2 analytically  !
! D85   D(18,13,14,19)          0.0            calculate D2E/DX2 analytically  !
! D86   D(18,13,21,1)          74.7635         calculate D2E/DX2 analytically  !
! D87   D(18,13,21,2)          40.9151         calculate D2E/DX2 analytically  !
! D88   D(18,13,21,3)           0.0            calculate D2E/DX2 analytically  !
! D89   D(18,13,21,4)         -40.9151         calculate D2E/DX2 analytically  !
! D90   D(18,13,21,5)         -74.7635         calculate D2E/DX2 analytically  !
! D91   D(18,13,21,11)        158.8139         calculate D2E/DX2 analytically  !
! D92   D(18,13,21,15)       -158.8139         calculate D2E/DX2 analytically  !
! D93   D(13,14,15,11)          0.0            calculate D2E/DX2 analytically  !
! D94   D(13,14,15,20)        177.1787         calculate D2E/DX2 analytically  !
! D95   D(19,14,15,11)       -177.1787         calculate D2E/DX2 analytically  !
! D96   D(19,14,15,20)          0.0            calculate D2E/DX2 analytically  !
! D97   D(19,14,21,1)          -74.7635         calculate D2E/DX2 analytically  !
! D98   D(19,14,21,2)           74.7635         calculate D2E/DX2 analytically  !
! D99   D(19,14,21,3)           40.9151         calculate D2E/DX2 analytically  !
```

```
 ! D100  D(19,14,21,4)          0.0           calculate D2E/DX2 analytically  !
 ! D101  D(19,14,21,5)        -40.9151        calculate D2E/DX2 analytically  !
 ! D102  D(19,14,21,11)      -158.8139        calculate D2E/DX2 analytically  !
 ! D103  D(19,14,21,12)       158.8139        calculate D2E/DX2 analytically  !
 ! D104  D(20,15,21,1)        -40.9151        calculate D2E/DX2 analytically  !
 ! D105  D(20,15,21,2)        -74.7635        calculate D2E/DX2 analytically  !
 ! D106  D(20,15,21,3)         74.7635        calculate D2E/DX2 analytically  !
 ! D107  D(20,15,21,4)         40.9151        calculate D2E/DX2 analytically  !
 ! D108  D(20,15,21,5)          0.0           calculate D2E/DX2 analytically  !
 ! D109  D(20,15,21,12)      -158.8139        calculate D2E/DX2 analytically  !
 ! D110  D(20,15,21,13)       158.8139        calculate D2E/DX2 analytically  !
 ---------------------------------------------------------------------------
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06 EigMax=2.50D+02
EigMin=1.00D-04
 Number of steps in this run=    126 maximum allowed number of steps=    126.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        0.000000    1.224974   -1.883463
      2          6           0       -1.165019    0.378538   -1.883463
      3          6           0       -0.720022   -0.991025   -1.883463
      4          6           0        0.720022   -0.991025   -1.883463
      5          6           0        1.165019    0.378538   -1.883463
      6          1           0       -2.189806    0.711511   -1.926423
      7          1           0       -1.353374   -1.862760   -1.926423
      8          1           0        1.353374   -1.862760   -1.926423
      9          1           0        2.189806    0.711511   -1.926423
     10          1           0        0.000000    2.302498   -1.926423
     11          6           0        0.000000    1.224974    1.883463
     12          6           0       -1.165019    0.378538    1.883463
     13          6           0       -0.720022   -0.991025    1.883463
     14          6           0        0.720022   -0.991025    1.883463
     15          6           0        1.165019    0.378538    1.883463
     16          1           0        0.000000    2.302498    1.926423
     17          1           0       -2.189806    0.711511    1.926423
     18          1           0       -1.353374   -1.862760    1.926423
     19          1           0        1.353374   -1.862760    1.926423
     20          1           0        2.189806    0.711511    1.926423
     21         44           0        0.000000    0.000000    0.000000
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                      1          2          3          4          5
    1  C    0.000000
    2  C    1.440043   0.000000
    3  C    2.330039   1.440043   0.000000
    4  C    2.330039   2.330039   1.440043   0.000000
```

5	C	1.440043	2.330039	2.330039	1.440043	0.000000
6	H	2.249609	1.078380	2.249609	3.371582	3.371582
7	H	3.371582	2.249609	1.078380	2.249609	3.371582
8	H	3.371582	3.371582	2.249609	1.078380	2.249609
9	H	2.249609	3.371582	3.371582	2.249609	1.078380
10	H	1.078380	2.249609	3.371582	3.371582	2.249609
11	C	3.766925	4.032797	4.429312	4.429312	4.032797
12	C	4.032797	3.766925	4.032797	4.429312	4.429312
13	C	4.429312	4.032797	3.766925	4.032797	4.429312
14	C	4.429312	4.429312	4.032797	3.766925	4.032797
15	C	4.032797	4.429312	4.429312	4.032797	3.766925
16	H	3.959329	4.424265	5.087332	5.087332	4.424265
17	H	4.424265	3.959329	4.424265	5.087332	5.087332
18	H	5.087332	4.424265	3.959329	4.424265	5.087332
19	H	5.087332	5.087332	4.424265	3.959329	4.424265
20	H	4.424265	5.087332	5.087332	4.424265	3.959329
21	Ru	2.246774	2.246774	2.246774	2.246774	2.246774

		6	7	8	9	10
6	H	0.000000				
7	H	2.706749	0.000000			
8	H	4.379611	2.706749	0.000000		
9	H	4.379611	4.379611	2.706749	0.000000	
10	H	2.706749	4.379611	4.379611	2.706749	0.000000
11	C	4.424265	5.087332	5.087332	4.424265	3.959329
12	C	3.959329	4.424265	5.087332	5.087332	4.424265
13	C	4.424265	3.959329	4.424265	5.087332	5.087332
14	C	5.087332	4.424265	3.959329	4.424265	5.087332
15	C	5.087332	5.087332	4.424265	3.959329	4.424265
16	H	4.708600	5.833131	5.833131	4.708600	3.852846
17	H	3.852846	4.708600	5.833131	5.833131	4.708600
18	H	4.708600	3.852846	4.708600	5.833131	5.833131
19	H	5.833131	4.708600	3.852846	4.708600	5.833131
20	H	5.833131	5.833131	4.708600	3.852846	4.708600
21	Ru	3.002100	3.002100	3.002100	3.002100	3.002100

		11	12	13	14	15
11	C	0.000000				
12	C	1.440043	0.000000			
13	C	2.330039	1.440043	0.000000		
14	C	2.330039	2.330039	1.440043	0.000000	
15	C	1.440043	2.330039	2.330039	1.440043	0.000000
16	H	1.078380	2.249609	3.371582	3.371582	2.249609
17	H	2.249609	1.078380	2.249609	3.371582	3.371582
18	H	3.371582	2.249609	1.078380	2.249609	3.371582
19	H	3.371582	3.371582	2.249609	1.078380	2.249609
20	H	2.249609	3.371582	3.371582	2.249609	1.078380
21	Ru	2.246774	2.246774	2.246774	2.246774	2.246774

		16	17	18	19	20
16	H	0.000000				
17	H	2.706749	0.000000			
18	H	4.379611	2.706749	0.000000		

```
   19  H    4.379611   4.379611   2.706749   0.000000
   20  H    2.706749   4.379611   4.379611   2.706749   0.000000
   21  Ru   3.002100   3.002100   3.002100   3.002100   3.002100
                  21
   21  Ru   0.000000
 Symm:  InNGrp=D5H  InAxis=0 RotPrA=F RotCs=T.
 This structure is nearly, but not quite of a higher symmetry.
 Consider Symm=Loose if the higher symmetry is desired.
 Stoichiometry    C10H10Ru
 Framework group  C1[X(C10H10Ru)]
 Deg. of freedom    57
 Full point group                 C1      NOp   1
 Largest Abelian subgroup         C1      NOp   1
 Largest concise Abelian subgroup C1      NOp   1
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.883463    1.224974    0.000001
      2          6           0       -1.883463    0.378537    1.165020
      3          6           0       -1.883463   -0.991025    0.720021
      4          6           0       -1.883463   -0.991024   -0.720022
      5          6           0       -1.883463    0.378539   -1.165019
      6          1           0       -1.926423    0.711510    2.189806
      7          1           0       -1.926423   -1.862761    1.353373
      8          1           0       -1.926423   -1.862759   -1.353375
      9          1           0       -1.926423    0.711512   -2.189805
     10          1           0       -1.926423    2.302498    0.000001
     11          6           0        1.883463    1.224974    0.000001
     12          6           0        1.883463    0.378537    1.165020
     13          6           0        1.883463   -0.991025    0.720021
     14          6           0        1.883463   -0.991024   -0.720022
     15          6           0        1.883463    0.378539   -1.165019
     16          1           0        1.926423    2.302498    0.000001
     17          1           0        1.926423    0.711510    2.189806
     18          1           0        1.926423   -1.862761    1.353373
     19          1           0        1.926423   -1.862759   -1.353375
     20          1           0        1.926423    0.711512   -2.189805
     21         44           0        0.000000    0.000000    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.1643904           0.8715809
0.8715809
 Standard basis: 3-21G* (6D, 7F)
 There are   149 symmetry adapted cartesian basis functions of A   symmetry.
 There are   149 symmetry adapted basis functions of A   symmetry.
   149 basis functions,   267 primitive gaussians,   149 cartesian basis functions
    57 alpha electrons       57 beta electrons
       nuclear repulsion energy      1146.1765810147 Hartrees.
 NAtoms=   21 NActive=   21 NUniq=   21 SFac= 1.00D+00 NAtFMM=   60 NAOKFM=F Big=F
```

```
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=   149 RedAO= T EigKep=  1.33D-03  NBF=   149
 NBsUse=   149 1.00D-06 EigRej= -1.00D+00 NBFU=   149
 Defaulting to unpruned grid for atomic number  44.
 ExpMin= 3.01D-02 ExpMax= 9.79D+03 ExpMxC= 9.79D+03 IAcc=3 IRadAn=         5
AccDes= 0.00D+00
 Harris functional with IExCor=  402 and IRadAn=       5 diagonalized for initial
guess.
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=  3500011 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Defaulting to unpruned grid for atomic number  44.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         wScrn=  0.000000 ICntrl=       500 IOpCl=  0 I1Cent=   200000004 NGrid=
       0
         NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=
  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.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
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 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 EnCoef did   100 forward-backward iterations
 SCF Done:  E(RB3LYP) =  -4808.20577746     A.U. after   11 cycles
            NFock= 11  Conv=0.90D-08     -V/T= 2.0049
 DoSCS=F DFT=T ScalE2(SS,OS)=  1.000000  1.000000
 Range of M.O.s used for correlation:     1   149
 NBasis=   149 NAE=    57 NBE=    57 NFC=     0 NFV=     0
 NROrb=    149 NOA=    57 NOB=    57 NVA=    92 NVB=    92

 **** Warning!!: The largest alpha MO coefficient is  0.20105565D+02
```

```
 Symmetrizing basis deriv contribution to polar:
 IMax=3 JMax=2 DiffMx= 0.00D+00
 G2DrvN: will do    22 centers at a time, making    1 passes.
 Calling FoFCou, ICntrl=  3107 FMM=F I1Cent=   0 AccDes= 0.00D+00.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
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 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 End of G2Drv F.D. properties file   721 does not exist.
 End of G2Drv F.D. properties file   722 does not exist.
 End of G2Drv F.D. properties file   788 does not exist.
          IDoAtm=11111111111111111111
          Differentiating once with respect to nuclear coordinates.
 Defaulting to unpruned grid for atomic number  44.
 Keep R1 ints in memory in canonical form, NReq=78040536.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
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 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
          There are    66 degrees of freedom in the 1st order CPHF.  IDoFFX=6
NUNeed=     0.
     60 vectors produced by pass  0 Test12= 7.95D-15 1.52D-09 XBig12= 9.97D-02
8.14D-02.
 AX will form    60 AO Fock derivatives at one time.
     60 vectors produced by pass  1 Test12= 7.95D-15 1.52D-09 XBig12= 1.83D-02
```

```
4.80D-02.
     60 vectors produced by pass  2 Test12= 7.95D-15 1.52D-09 XBig12= 1.31D-04
2.41D-03.
     60 vectors produced by pass  3 Test12= 7.95D-15 1.52D-09 XBig12= 7.37D-07
2.96D-04.
     60 vectors produced by pass  4 Test12= 7.95D-15 1.52D-09 XBig12= 1.34D-09
9.30D-06.
     60 vectors produced by pass  5 Test12= 7.95D-15 1.52D-09 XBig12= 1.53D-12
2.83D-07.
     11 vectors produced by pass  6 Test12= 7.95D-15 1.52D-09 XBig12= 2.53D-15
9.96D-09.
 InvSVY:  IOpt=1 It=  1 EMax= 2.78D-16
 Solved reduced A of dimension   371 with    66 vectors.
 End of Minotr F.D. properties file   721 does not exist.
 End of Minotr F.D. properties file   722 does not exist.
 End of Minotr F.D. properties file   788 does not exist.

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

           Population analysis using the SCF Density.

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

 Orbital symmetries:
       Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A)
 The electronic state is 1-A.
 Alpha  occ. eigenvalues -- -781.88987-111.30451-102.62951-102.62282-102.62282
 Alpha  occ. eigenvalues --  -19.87367 -16.30147 -16.28637 -16.28637 -10.49042
 Alpha  occ. eigenvalues --  -10.48816 -10.48816 -10.47829 -10.47829 -10.13575
 Alpha  occ. eigenvalues --  -10.13575 -10.13545 -10.13545 -10.13540 -10.13539
 Alpha  occ. eigenvalues --  -10.13539 -10.13516 -10.13516 -10.13454  -2.74356
 Alpha  occ. eigenvalues --   -1.69701  -1.64619  -1.64619  -0.88958  -0.87264
 Alpha  occ. eigenvalues --   -0.71485  -0.71485  -0.70845  -0.70845  -0.54673
 Alpha  occ. eigenvalues --   -0.54673  -0.54239  -0.54239  -0.53730  -0.52612
 Alpha  occ. eigenvalues --   -0.41576  -0.41576  -0.40439  -0.40439  -0.40056
 Alpha  occ. eigenvalues --   -0.38171  -0.38171  -0.37957  -0.37957  -0.35489
 Alpha  occ. eigenvalues --   -0.28656  -0.28656  -0.23020  -0.23020  -0.21002
 Alpha  occ. eigenvalues --   -0.19397  -0.19397
```

```
Alpha virt. eigenvalues --   -0.00195  -0.00195   0.02674   0.03552   0.03553
Alpha virt. eigenvalues --    0.05363   0.05966   0.05966   0.08746   0.08746
Alpha virt. eigenvalues --    0.16813   0.17440   0.18617   0.18617   0.19402
Alpha virt. eigenvalues --    0.19402   0.19553   0.19553   0.20372   0.20374
Alpha virt. eigenvalues --    0.24684   0.24684   0.25190   0.25190   0.25893
Alpha virt. eigenvalues --    0.31000   0.31000   0.39011   0.39011   0.39608
Alpha virt. eigenvalues --    0.39608   0.44259   0.44600   0.44880   0.50271
Alpha virt. eigenvalues --    0.69657   0.69657   0.71633   0.71633   0.71714
Alpha virt. eigenvalues --    0.71714   0.76761   0.77130   0.77832   0.77832
Alpha virt. eigenvalues --    0.79768   0.79768   0.83880   0.83880   0.86477
Alpha virt. eigenvalues --    0.88184   0.88184   0.91362   0.96775   0.96776
Alpha virt. eigenvalues --    0.98174   0.98174   0.98757   0.98757   1.00969
Alpha virt. eigenvalues --    1.01999   1.05437   1.05437   1.10319   1.10319
Alpha virt. eigenvalues --    1.17720   1.19752   1.20216   1.20216   1.26160
Alpha virt. eigenvalues --    1.26160   1.34726   1.34726   1.36731   1.37604
Alpha virt. eigenvalues --    1.37604   1.38899   1.38900   1.39618   1.39618
Alpha virt. eigenvalues --    1.93556   2.00504   2.00505   2.02444   2.02444
Alpha virt. eigenvalues --    2.28875   2.42659   2.42659   2.43733   2.43733
Alpha virt. eigenvalues --    3.24387 152.27236
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C    5.473624   0.360191  -0.118532  -0.118532   0.360191  -0.028544
     2  C    0.360191   5.473629   0.360192  -0.118532  -0.118533   0.399486
     3  C   -0.118532   0.360192   5.473619   0.360190  -0.118532  -0.028544
     4  C   -0.118532  -0.118532   0.360190   5.473619   0.360192   0.003143
     5  C    0.360191  -0.118533  -0.118532   0.360192   5.473629   0.003143
     6  H   -0.028544   0.399486  -0.028544   0.003143   0.003143   0.459811
     7  H    0.003143  -0.028545   0.399487  -0.028544   0.003143  -0.001535
     8  H    0.003143   0.003143  -0.028544   0.399487  -0.028545  -0.000018
     9  H   -0.028544   0.003143   0.003143  -0.028544   0.399486  -0.000018
    10  H    0.399486  -0.028544   0.003143   0.003143  -0.028544  -0.001535
    11  C    0.008246  -0.001791  -0.000649  -0.000649  -0.001791  -0.000036
    12  C   -0.001791   0.008246  -0.001791  -0.000649  -0.000649  -0.000281
    13  C   -0.000649  -0.001791   0.008246  -0.001791  -0.000649  -0.000036
    14  C   -0.000649  -0.000649  -0.001791   0.008246  -0.001791   0.000000
    15  C   -0.001791  -0.000649  -0.000649  -0.001791   0.008246   0.000000
    16  H   -0.000281  -0.000036   0.000000   0.000000  -0.000036   0.000001
    17  H   -0.000036  -0.000281  -0.000036   0.000000   0.000000   0.000007
    18  H    0.000000  -0.000036  -0.000281  -0.000036   0.000000   0.000001
    19  H    0.000000   0.000000  -0.000036  -0.000281  -0.000036   0.000000
    20  H   -0.000036   0.000000   0.000000  -0.000036  -0.000281   0.000000
    21  Ru  -0.014226  -0.014233  -0.014227  -0.014227  -0.014233  -0.005721
               7          8          9         10         11         12
     1  C    0.003143   0.003143  -0.028544   0.399486   0.008246  -0.001791
     2  C   -0.028545   0.003143   0.003143  -0.028544  -0.001791   0.008246
     3  C    0.399487  -0.028544   0.003143   0.003143  -0.000649  -0.001791
     4  C   -0.028544   0.399487  -0.028544   0.003143  -0.000649  -0.000649
     5  C    0.003143  -0.028545   0.399486  -0.028544  -0.001791  -0.000649
     6  H   -0.001535  -0.000018  -0.000018  -0.001535  -0.000036  -0.000281
     7  H    0.459810  -0.001535  -0.000018  -0.000018   0.000000  -0.000036
```

8	H	-0.001535	0.459810	-0.001535	-0.000018	0.000000	0.000000
9	H	-0.000018	-0.001535	0.459811	-0.001535	-0.000036	0.000000
10	H	-0.000018	-0.000018	-0.001535	0.459810	-0.000281	-0.000036
11	C	0.000000	0.000000	-0.000036	-0.000281	5.473624	0.360191
12	C	-0.000036	0.000000	0.000000	-0.000036	0.360191	5.473629
13	C	-0.000281	-0.000036	0.000000	0.000000	-0.118532	0.360192
14	C	-0.000036	-0.000281	-0.000036	0.000000	-0.118532	-0.118532
15	C	0.000000	-0.000036	-0.000281	-0.000036	0.360191	-0.118533
16	H	0.000000	0.000000	0.000001	0.000007	0.399486	-0.028544
17	H	0.000001	0.000000	0.000000	0.000001	-0.028544	0.399486
18	H	0.000007	0.000001	0.000000	0.000000	0.003143	-0.028545
19	H	0.000001	0.000007	0.000001	0.000000	0.003143	0.003143
20	H	0.000000	0.000001	0.000007	0.000001	-0.028544	0.003143
21	Ru	-0.005721	-0.005721	-0.005721	-0.005721	-0.014226	-0.014233

		13	14	15	16	17	18
1	C	-0.000649	-0.000649	-0.001791	-0.000281	-0.000036	0.000000
2	C	-0.001791	-0.000649	-0.000649	-0.000036	-0.000281	-0.000036
3	C	0.008246	-0.001791	-0.000649	0.000000	-0.000036	-0.000281
4	C	-0.001791	0.008246	-0.001791	0.000000	0.000000	-0.000036
5	C	-0.000649	-0.001791	0.008246	-0.000036	0.000000	0.000000
6	H	-0.000036	0.000000	0.000000	0.000001	0.000007	0.000001
7	H	-0.000281	-0.000036	0.000000	0.000000	0.000001	0.000007
8	H	-0.000036	-0.000281	-0.000036	0.000000	0.000000	0.000001
9	H	0.000000	-0.000036	-0.000281	0.000001	0.000000	0.000000
10	H	0.000000	0.000000	-0.000036	0.000007	0.000001	0.000000
11	C	-0.118532	-0.118532	0.360191	0.399486	-0.028544	0.003143
12	C	0.360192	-0.118532	-0.118533	-0.028544	0.399486	-0.028545
13	C	5.473619	0.360190	-0.118532	0.003143	-0.028544	0.399487
14	C	0.360190	5.473619	0.360192	0.003143	0.003143	-0.028544
15	C	-0.118532	0.360192	5.473629	-0.028544	0.003143	0.003143
16	H	0.003143	0.003143	-0.028544	0.459810	-0.001535	-0.000018
17	H	-0.028544	0.003143	0.003143	-0.001535	0.459811	-0.001535
18	H	0.399487	-0.028544	0.003143	-0.000018	-0.001535	0.459810
19	H	-0.028544	0.399487	-0.028545	-0.000018	-0.000018	-0.001535
20	H	0.003143	-0.028544	0.399486	-0.001535	-0.000018	-0.000018
21	Ru	-0.014227	-0.014227	-0.014233	-0.005721	-0.005721	-0.005721

		19	20	21
1	C	0.000000	-0.000036	-0.014226
2	C	0.000000	0.000000	-0.014233
3	C	-0.000036	0.000000	-0.014227
4	C	-0.000281	-0.000036	-0.014227
5	C	-0.000036	-0.000281	-0.014233
6	H	0.000000	0.000000	-0.005721
7	H	0.000001	0.000000	-0.005721
8	H	0.000007	0.000001	-0.005721
9	H	0.000001	0.000007	-0.005721
10	H	0.000000	0.000001	-0.005721
11	C	0.003143	-0.028544	-0.014226
12	C	0.003143	0.003143	-0.014233
13	C	-0.028544	0.003143	-0.014227

```
   14  C    0.399487  -0.028544  -0.014227
   15  C   -0.028545   0.399486  -0.014233
   16  H   -0.000018  -0.001535  -0.005721
   17  H   -0.000018  -0.000018  -0.005721
   18  H   -0.001535  -0.000018  -0.005721
   19  H    0.459810  -0.001535  -0.005721
   20  H   -0.001535   0.459811  -0.005721
   21  Ru  -0.005721  -0.005721  43.262165
Mulliken charges:
              1
    1  C   -0.294412
    2  C   -0.294411
    3  C   -0.294407
    4  C   -0.294407
    5  C   -0.294411
    6  H    0.200675
    7  H    0.200676
    8  H    0.200676
    9  H    0.200675
   10  H    0.200677
   11  C   -0.294412
   12  C   -0.294411
   13  C   -0.294407
   14  C   -0.294407
   15  C   -0.294411
   16  H    0.200677
   17  H    0.200675
   18  H    0.200676
   19  H    0.200676
   20  H    0.200675
   21  Ru   0.937338
Sum of Mulliken charges =  -0.00000
Mulliken charges with hydrogens summed into heavy atoms:
              1
    1  C   -0.093735
    2  C   -0.093736
    3  C   -0.093731
    4  C   -0.093731
    5  C   -0.093736
   11  C   -0.093735
   12  C   -0.093736
   13  C   -0.093731
   14  C   -0.093731
   15  C   -0.093736
   21  Ru   0.937338
APT charges:
              1
    1  C   -0.755606
    2  C   -0.755612
    3  C   -0.755611
```

```
     4  C   -0.755611
     5  C   -0.755612
     6  H    0.597767
     7  H    0.597768
     8  H    0.597768
     9  H    0.597767
    10  H    0.597766
    11  C   -0.755606
    12  C   -0.755612
    13  C   -0.755611
    14  C   -0.755611
    15  C   -0.755612
    16  H    0.597766
    17  H    0.597767
    18  H    0.597768
    19  H    0.597768
    20  H    0.597767
    21  Ru   1.578429
 Sum of APT charges =  -0.00000
 APT charges with hydrogens summed into heavy atoms:
               1
     1  C   -0.157840
     2  C   -0.157844
     3  C   -0.157843
     4  C   -0.157843
     5  C   -0.157844
    11  C   -0.157840
    12  C   -0.157844
    13  C   -0.157843
    14  C   -0.157843
    15  C   -0.157844
    21  Ru   1.578429
 Electronic spatial extent (au):  <R**2>=           1580.3478
 Charge=              -0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=              0.0000    Y=              0.0000    Z=             -0.0000
Tot=              0.0000
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=            -87.9302   YY=            -75.0029   ZZ=            -75.0027
   XY=              0.0000   XZ=              0.0000   YZ=              0.0000
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=             -8.6183   YY=              4.3091   ZZ=              4.3093
   XY=              0.0000   XZ=              0.0000   YZ=              0.0000
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=              0.0000  YYY=             -0.0001  ZZZ=             -0.0000
XYY=             -0.0000
  XXY=             -0.0001  XXZ=              0.0000  XZZ=             -0.0000
YZZ=             -0.0001
  YYZ=             -0.0000  XYZ=              0.0000
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
```

```
 XXXX=          -1523.7126 YYYY=           -384.4330 ZZZZ=           -384.4311
XXXY=              0.0000
 XXXZ=              0.0000 YYYX=              0.0000 YYYZ=              0.0000
ZZZX=              0.0000
 ZZZY=              0.0000 XXYY=           -275.0290 XXZZ=           -275.0296
YYZZ=           -128.1440
 XXYZ=              0.0000 YYXZ=              0.0000 ZZXY=              0.0000
 N-N= 1.146176581015D+03 E-N=-1.369676257784D+04  KE= 4.784544668713D+03
  Exact polarizability:   0.000   0.000   0.000   0.000   0.000   0.000
 Approx polarizability: 264.450   0.000 175.218   0.000  -0.000 175.216
 Calling FoFJK, ICntrl=    100147 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
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 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                   Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1        6           0.000000000   -0.000000092    0.000007779
      2        6           0.000001262   -0.000002837   -0.000001367
      3        6           0.000002679    0.000007303   -0.000002000
      4        6          -0.000002679    0.000007303   -0.000002000
      5        6          -0.000001262   -0.000002837   -0.000001367
      6        1           0.000009296   -0.000002041    0.000001557
      7        1           0.000007415    0.000004991    0.000000720
      8        1          -0.000007415    0.000004991    0.000000720
      9        1          -0.000009296   -0.000002041    0.000001557
     10        1           0.000000000   -0.000013061   -0.000003631
     11        6           0.000000000   -0.000000092   -0.000007779
     12        6           0.000001262   -0.000002837    0.000001367
     13        6           0.000002679    0.000007303    0.000002000
     14        6          -0.000002679    0.000007303    0.000002000
     15        6          -0.000001262   -0.000002837    0.000001367
     16        1           0.000000000   -0.000013061    0.000003631
     17        1           0.000009296   -0.000002041   -0.000001557
```

```
    18        1           0.000007415    0.000004991   -0.000000720
    19        1          -0.000007415    0.000004991   -0.000000720
    20        1          -0.000009296   -0.000002041   -0.000001557
    21       44          -0.000000000   -0.000003359   -0.000000000
---------------------------------------------------------------------
Cartesian Forces:  Max     0.000013061 RMS     0.000004876
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000012906 RMS     0.000003023
Search for a local minimum.
Step number   1 out of a maximum of  126
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Second derivative matrix not updated -- analytic derivatives used.
ITU=  0
    Eigenvalues ---    0.00065   0.00217   0.00220   0.01019   0.01019
    Eigenvalues ---    0.01048   0.01049   0.01260   0.01260   0.01304
    Eigenvalues ---    0.01305   0.01343   0.01343   0.01454   0.01454
    Eigenvalues ---    0.01476   0.01679   0.01749   0.01750   0.02050
    Eigenvalues ---    0.02050   0.02305   0.02360   0.03087   0.03423
    Eigenvalues ---    0.03423   0.03706   0.03709   0.05682   0.06872
    Eigenvalues ---    0.06875   0.07333   0.07353   0.11772   0.11773
    Eigenvalues ---    0.14135   0.14136   0.19669   0.20976   0.20981
    Eigenvalues ---    0.21603   0.21609   0.23063   0.23064   0.26143
    Eigenvalues ---    0.26145   0.30219   0.37565   0.37566   0.37592
    Eigenvalues ---    0.37592   0.37628   0.37630   0.37639   0.37640
    Eigenvalues ---    0.37724   0.37731
RFO step:  Lambda= 0.00000000D+00 EMin= 6.53756558D-04
Linear search not attempted -- first point.
Iteration  1 RMS(Cart)=  0.00002907 RMS(Int)=  0.00000000
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.72129  -0.00001   0.00000  -0.00002  -0.00002   2.72127
   R2        2.72129  -0.00001   0.00000  -0.00002  -0.00002   2.72127
   R3        2.03784  -0.00001   0.00000  -0.00003  -0.00003   2.03781
   R4        4.24579  -0.00000   0.00000  -0.00006  -0.00006   4.24572
   R5        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72125
   R6        2.03784  -0.00001   0.00000  -0.00003  -0.00003   2.03782
   R7        4.24579  -0.00000   0.00000  -0.00001  -0.00001   4.24578
   R8        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
   R9        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
  R10        4.24579  -0.00000   0.00000   0.00002   0.00002   4.24581
  R11        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72125
  R12        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
  R13        4.24579  -0.00000   0.00000   0.00002   0.00002   4.24581
  R14        2.03784  -0.00001   0.00000  -0.00003  -0.00003   2.03782
  R15        4.24579  -0.00000   0.00000  -0.00001  -0.00001   4.24578
```

R16	2.72129	-0.00001	0.00000	-0.00002	-0.00002	2.72127
R17	2.72129	-0.00001	0.00000	-0.00002	-0.00002	2.72127
R18	2.03784	-0.00001	0.00000	-0.00003	-0.00003	2.03781
R19	4.24579	-0.00000	0.00000	-0.00006	-0.00006	4.24572
R20	2.72129	-0.00001	0.00000	-0.00003	-0.00003	2.72125
R21	2.03784	-0.00001	0.00000	-0.00003	-0.00003	2.03782
R22	4.24579	-0.00000	0.00000	-0.00001	-0.00001	4.24578
R23	2.72129	-0.00001	0.00000	-0.00003	-0.00003	2.72126
R24	2.03784	-0.00001	0.00000	-0.00002	-0.00002	2.03782
R25	4.24579	-0.00000	0.00000	0.00002	0.00002	4.24581
R26	2.72129	-0.00001	0.00000	-0.00003	-0.00003	2.72125
R27	2.03784	-0.00001	0.00000	-0.00002	-0.00002	2.03782
R28	4.24579	-0.00000	0.00000	0.00002	0.00002	4.24581
R29	2.03784	-0.00001	0.00000	-0.00003	-0.00003	2.03782
R30	4.24579	-0.00000	0.00000	-0.00001	-0.00001	4.24578
A1	1.88496	0.00000	0.00000	0.00000	0.00000	1.88496
A2	2.19854	-0.00000	0.00000	-0.00000	-0.00000	2.19853
A3	2.19854	-0.00000	0.00000	-0.00000	-0.00000	2.19853
A4	2.18729	-0.00000	0.00000	0.00007	0.00007	2.18736
A5	1.88496	-0.00000	0.00000	-0.00001	-0.00001	1.88495
A6	2.19854	0.00000	0.00000	-0.00001	-0.00001	2.19853
A7	2.19854	0.00000	0.00000	0.00002	0.00002	2.19855
A8	2.18729	-0.00000	0.00000	-0.00002	-0.00002	2.18727
A9	1.88496	0.00000	0.00000	0.00001	0.00001	1.88496
A10	2.19854	0.00000	0.00000	0.00003	0.00003	2.19857
A11	2.19854	-0.00000	0.00000	-0.00003	-0.00003	2.19850
A12	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A13	1.88496	0.00000	0.00000	0.00001	0.00001	1.88496
A14	2.19854	-0.00000	0.00000	-0.00003	-0.00003	2.19850
A15	2.19854	0.00000	0.00000	0.00003	0.00003	2.19857
A16	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A17	1.88496	-0.00000	0.00000	-0.00001	-0.00001	1.88495
A18	2.19854	0.00000	0.00000	-0.00001	-0.00001	2.19853
A19	2.19854	0.00000	0.00000	0.00002	0.00002	2.19855
A20	2.18729	-0.00000	0.00000	-0.00002	-0.00002	2.18727
A21	1.88496	0.00000	0.00000	0.00000	0.00000	1.88496
A22	2.19854	-0.00000	0.00000	-0.00000	-0.00000	2.19853
A23	2.19854	-0.00000	0.00000	-0.00000	-0.00000	2.19853
A24	2.18729	-0.00000	0.00000	0.00007	0.00007	2.18736
A25	1.88496	-0.00000	0.00000	-0.00001	-0.00001	1.88495
A26	2.19854	0.00000	0.00000	-0.00001	-0.00001	2.19853
A27	2.19854	0.00000	0.00000	0.00002	0.00002	2.19855
A28	2.18729	-0.00000	0.00000	-0.00002	-0.00002	2.18727
A29	1.88496	0.00000	0.00000	0.00001	0.00001	1.88496
A30	2.19854	0.00000	0.00000	0.00003	0.00003	2.19857
A31	2.19854	-0.00000	0.00000	-0.00003	-0.00003	2.19850
A32	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A33	1.88496	0.00000	0.00000	0.00001	0.00001	1.88496
A34	2.19854	-0.00000	0.00000	-0.00003	-0.00003	2.19850
A35	2.19854	0.00000	0.00000	0.00003	0.00003	2.19857

A36	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A37	1.88496	-0.00000	0.00000	-0.00001	-0.00001	1.88495
A38	2.19854	0.00000	0.00000	-0.00001	-0.00001	2.19853
A39	2.19854	0.00000	0.00000	0.00002	0.00002	2.19855
A40	2.18729	-0.00000	0.00000	-0.00002	-0.00002	2.18727
A41	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A42	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A43	1.98830	0.00000	0.00000	-0.00004	-0.00004	1.98826
A44	2.22797	0.00000	0.00000	-0.00003	-0.00003	2.22794
A45	2.80302	0.00000	0.00000	-0.00001	-0.00001	2.80301
A46	2.80302	0.00000	0.00000	-0.00001	-0.00001	2.80301
A47	2.22797	0.00000	0.00000	-0.00003	-0.00003	2.22794
A48	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A49	1.09026	-0.00000	0.00000	-0.00000	-0.00000	1.09026
A50	2.22797	0.00000	0.00000	-0.00003	-0.00003	2.22794
A51	1.98830	0.00000	0.00000	-0.00001	-0.00001	1.98830
A52	2.22797	0.00000	0.00000	0.00002	0.00002	2.22799
A53	2.80302	0.00000	0.00000	0.00003	0.00003	2.80305
A54	2.80302	0.00000	0.00000	-0.00003	-0.00003	2.80299
A55	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A56	2.80302	0.00000	0.00000	-0.00001	-0.00001	2.80301
A57	2.22797	0.00000	0.00000	0.00002	0.00002	2.22799
A58	1.98830	0.00000	0.00000	0.00005	0.00005	1.98836
A59	2.22797	0.00000	0.00000	0.00005	0.00005	2.22803
A60	2.80302	0.00000	0.00000	0.00003	0.00003	2.80305
A61	2.80302	0.00000	0.00000	-0.00001	-0.00001	2.80301
A62	2.80302	0.00000	0.00000	0.00003	0.00003	2.80305
A63	2.22797	0.00000	0.00000	0.00005	0.00005	2.22803
A64	1.98830	0.00000	0.00000	0.00005	0.00005	1.98836
A65	2.22797	0.00000	0.00000	0.00002	0.00002	2.22799
A66	2.22797	0.00000	0.00000	-0.00003	-0.00003	2.22794
A67	2.80302	0.00000	0.00000	-0.00003	-0.00003	2.80299
A68	2.80302	0.00000	0.00000	0.00003	0.00003	2.80305
A69	2.22797	0.00000	0.00000	0.00002	0.00002	2.22799
A70	1.98830	0.00000	0.00000	-0.00001	-0.00001	1.98830
A71	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A72	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A73	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A74	1.09026	-0.00000	0.00000	-0.00000	-0.00000	1.09026
A75	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
D1	0.00000	0.00000	0.00000	0.00002	0.00002	0.00002
D2	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09236
D3	3.09235	-0.00000	0.00000	-0.00011	-0.00011	3.09224
D4	0.00000	-0.00000	0.00000	-0.00014	-0.00014	-0.00014
D5	0.00000	-0.00000	0.00000	-0.00002	-0.00002	-0.00002
D6	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09236
D7	-3.09235	0.00000	0.00000	0.00011	0.00011	-3.09224
D8	-0.00000	0.00000	0.00000	0.00014	0.00014	0.00014
D9	2.77183	0.00000	0.00000	0.00000	0.00000	2.77183
D10	-2.77183	-0.00000	0.00000	-0.00000	-0.00000	-2.77183

D11	-0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000
D12	0.71410	-0.00000	0.00000	-0.00002	-0.00002	0.71408
D13	1.30487	-0.00000	0.00000	-0.00014	-0.00014	1.30472
D14	-1.30487	0.00000	0.00000	0.00014	0.00014	-1.30472
D15	-0.71410	0.00000	0.00000	0.00002	0.00002	-0.71408
D16	0.00000	-0.00000	0.00000	-0.00001	-0.00001	-0.00001
D17	-3.09235	0.00000	0.00000	-0.00002	-0.00002	-3.09237
D18	3.09235	-0.00000	0.00000	0.00002	0.00002	3.09237
D19	0.00000	-0.00000	0.00000	0.00001	0.00001	0.00001
D20	2.77183	0.00000	0.00000	0.00002	0.00002	2.77185
D21	-2.77183	-0.00000	0.00000	0.00001	0.00001	-2.77181
D22	-0.71410	0.00000	0.00000	-0.00002	-0.00002	-0.71412
D23	-0.00000	0.00000	0.00000	-0.00002	-0.00002	-0.00002
D24	0.71410	-0.00000	0.00000	-0.00004	-0.00004	0.71407
D25	1.30487	-0.00000	0.00000	-0.00008	-0.00008	1.30478
D26	-1.30487	0.00000	0.00000	0.00001	0.00001	-1.30486
D27	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000
D28	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09237
D29	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09237
D30	-0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000
D31	-2.77183	-0.00000	0.00000	-0.00004	-0.00004	-2.77186
D32	2.77183	-0.00000	0.00000	-0.00005	-0.00005	2.77178
D33	-1.30487	-0.00000	0.00000	-0.00019	-0.00019	-1.30506
D34	-0.71410	-0.00000	0.00000	-0.00008	-0.00008	-0.71419
D35	-0.00000	-0.00000	0.00000	-0.00006	-0.00006	-0.00006
D36	0.71410	-0.00000	0.00000	-0.00005	-0.00005	0.71405
D37	1.30487	-0.00000	0.00000	0.00004	0.00004	1.30491
D38	0.00000	0.00000	0.00000	0.00001	0.00001	0.00001
D39	-3.09235	0.00000	0.00000	-0.00002	-0.00002	-3.09237
D40	3.09235	-0.00000	0.00000	0.00002	0.00002	3.09237
D41	-0.00000	0.00000	0.00000	-0.00001	-0.00001	-0.00001
D42	2.77183	0.00000	0.00000	0.00004	0.00004	2.77186
D43	-2.77183	0.00000	0.00000	0.00005	0.00005	-2.77178
D44	1.30487	0.00000	0.00000	0.00019	0.00019	1.30506
D45	-1.30487	0.00000	0.00000	-0.00004	-0.00004	-1.30491
D46	-0.71410	0.00000	0.00000	0.00005	0.00005	-0.71405
D47	0.00000	0.00000	0.00000	0.00006	0.00006	0.00006
D48	0.71410	0.00000	0.00000	0.00008	0.00008	0.71419
D49	2.77183	0.00000	0.00000	-0.00001	-0.00001	2.77181
D50	-2.77183	-0.00000	0.00000	-0.00002	-0.00002	-2.77185
D51	0.71410	-0.00000	0.00000	0.00002	0.00002	0.71412
D52	1.30487	-0.00000	0.00000	-0.00001	-0.00001	1.30486
D53	-1.30487	0.00000	0.00000	0.00008	0.00008	-1.30478
D54	-0.71410	0.00000	0.00000	0.00004	0.00004	-0.71407
D55	0.00000	-0.00000	0.00000	0.00002	0.00002	0.00002
D56	0.00000	-0.00000	0.00000	-0.00002	-0.00002	-0.00002
D57	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09236
D58	-3.09235	0.00000	0.00000	0.00011	0.00011	-3.09224
D59	-0.00000	0.00000	0.00000	0.00014	0.00014	0.00014
D60	0.00000	0.00000	0.00000	0.00002	0.00002	0.00002

D61	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09236
D62	3.09235	-0.00000	0.00000	-0.00011	-0.00011	3.09224
D63	0.00000	-0.00000	0.00000	-0.00014	-0.00014	-0.00014
D64	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D65	-0.71410	0.00000	0.00000	0.00002	0.00002	-0.71408
D66	-1.30487	0.00000	0.00000	0.00014	0.00014	-1.30472
D67	1.30487	-0.00000	0.00000	-0.00014	-0.00014	1.30472
D68	0.71410	-0.00000	0.00000	-0.00002	-0.00002	0.71408
D69	-2.77183	-0.00000	0.00000	-0.00000	-0.00000	-2.77183
D70	2.77183	0.00000	0.00000	0.00000	0.00000	2.77183
D71	0.00000	0.00000	0.00000	0.00001	0.00001	0.00001
D72	3.09235	-0.00000	0.00000	0.00002	0.00002	3.09237
D73	-3.09235	0.00000	0.00000	-0.00002	-0.00002	-3.09237
D74	-0.00000	0.00000	0.00000	-0.00001	-0.00001	-0.00001
D75	0.71410	-0.00000	0.00000	0.00002	0.00002	0.71412
D76	0.00000	-0.00000	0.00000	0.00002	0.00002	0.00002
D77	-0.71410	0.00000	0.00000	0.00004	0.00004	-0.71407
D78	-1.30487	0.00000	0.00000	0.00008	0.00008	-1.30478
D79	1.30487	-0.00000	0.00000	-0.00001	-0.00001	1.30486
D80	-2.77183	-0.00000	0.00000	-0.00002	-0.00002	-2.77185
D81	2.77183	0.00000	0.00000	-0.00001	-0.00001	2.77181
D82	0.00000	0.00000	0.00000	0.00000	-0.00000	0.00000
D83	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09237
D84	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09237
D85	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D86	1.30487	0.00000	0.00000	0.00019	0.00019	1.30506
D87	0.71410	0.00000	0.00000	0.00008	0.00008	0.71419
D88	0.00000	0.00000	0.00000	0.00006	0.00006	0.00006
D89	-0.71410	0.00000	0.00000	0.00005	0.00005	-0.71405
D90	-1.30487	0.00000	0.00000	-0.00004	-0.00004	-1.30491
D91	2.77183	0.00000	0.00000	0.00004	0.00004	2.77186
D92	-2.77183	0.00000	0.00000	0.00005	0.00005	-2.77178
D93	0.00000	-0.00000	0.00000	-0.00001	-0.00001	-0.00001
D94	3.09235	-0.00000	0.00000	0.00002	0.00002	3.09237
D95	-3.09235	0.00000	0.00000	-0.00002	-0.00002	-3.09237
D96	0.00000	-0.00000	0.00000	0.00001	0.00001	0.00001
D97	-1.30487	-0.00000	0.00000	-0.00019	-0.00019	-1.30506
D98	1.30487	-0.00000	0.00000	0.00004	0.00004	1.30491
D99	0.71410	-0.00000	0.00000	-0.00005	-0.00005	0.71405
D100	-0.00000	-0.00000	0.00000	-0.00006	-0.00006	-0.00006
D101	-0.71410	-0.00000	0.00000	-0.00008	-0.00008	-0.71419
D102	-2.77183	-0.00000	0.00000	-0.00004	-0.00004	-2.77186
D103	2.77183	-0.00000	0.00000	-0.00005	-0.00005	2.77178
D104	-0.71410	0.00000	0.00000	-0.00002	-0.00002	-0.71412
D105	-1.30487	0.00000	0.00000	0.00001	0.00001	-1.30486
D106	1.30487	-0.00000	0.00000	-0.00008	-0.00008	1.30478
D107	0.71410	-0.00000	0.00000	-0.00004	-0.00004	0.71407
D108	-0.00000	0.00000	0.00000	-0.00002	-0.00002	-0.00002
D109	-2.77183	-0.00000	0.00000	0.00001	0.00001	-2.77181
D110	2.77183	0.00000	0.00000	0.00002	0.00002	2.77185

```
         Item               Value     Threshold  Converged?
Maximum Force            0.000013     0.000450     YES
RMS     Force            0.000003     0.000300     YES
Maximum Displacement     0.000121     0.001800     YES
RMS     Displacement     0.000029     0.001200     YES
Predicted change in Energy=-4.665838D-09
Optimization completed.
   -- Stationary point found.
                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.44           -DE/DX =    0.0                 !
! R2    R(1,5)                  1.44           -DE/DX =    0.0                 !
! R3    R(1,10)                 1.0784         -DE/DX =    0.0                 !
! R4    R(1,21)                 2.2468         -DE/DX =    0.0                 !
! R5    R(2,3)                  1.44           -DE/DX =    0.0                 !
! R6    R(2,6)                  1.0784         -DE/DX =    0.0                 !
! R7    R(2,21)                 2.2468         -DE/DX =    0.0                 !
! R8    R(3,4)                  1.44           -DE/DX =    0.0                 !
! R9    R(3,7)                  1.0784         -DE/DX =    0.0                 !
! R10   R(3,21)                 2.2468         -DE/DX =    0.0                 !
! R11   R(4,5)                  1.44           -DE/DX =    0.0                 !
! R12   R(4,8)                  1.0784         -DE/DX =    0.0                 !
! R13   R(4,21)                 2.2468         -DE/DX =    0.0                 !
! R14   R(5,9)                  1.0784         -DE/DX =    0.0                 !
! R15   R(5,21)                 2.2468         -DE/DX =    0.0                 !
! R16   R(11,12)                1.44           -DE/DX =    0.0                 !
! R17   R(11,15)                1.44           -DE/DX =    0.0                 !
! R18   R(11,16)                1.0784         -DE/DX =    0.0                 !
! R19   R(11,21)                2.2468         -DE/DX =    0.0                 !
! R20   R(12,13)                1.44           -DE/DX =    0.0                 !
! R21   R(12,17)                1.0784         -DE/DX =    0.0                 !
! R22   R(12,21)                2.2468         -DE/DX =    0.0                 !
! R23   R(13,14)                1.44           -DE/DX =    0.0                 !
! R24   R(13,18)                1.0784         -DE/DX =    0.0                 !
! R25   R(13,21)                2.2468         -DE/DX =    0.0                 !
! R26   R(14,15)                1.44           -DE/DX =    0.0                 !
! R27   R(14,19)                1.0784         -DE/DX =    0.0                 !
! R28   R(14,21)                2.2468         -DE/DX =    0.0                 !
! R29   R(15,20)                1.0784         -DE/DX =    0.0                 !
! R30   R(15,21)                2.2468         -DE/DX =    0.0                 !
! A1    A(2,1,5)                108.0          -DE/DX =    0.0                 !
! A2    A(2,1,10)               125.967        -DE/DX =    0.0                 !
! A3    A(5,1,10)               125.967        -DE/DX =    0.0                 !
! A4    A(10,1,21)              125.3225       -DE/DX =    0.0                 !
! A5    A(1,2,3)                108.0          -DE/DX =    0.0                 !
! A6    A(1,2,6)                125.967        -DE/DX =    0.0                 !
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! A7    A(3,2,6)             125.967          -DE/DX =    0.0                !
! A8    A(6,2,21)            125.3225         -DE/DX =    0.0                !
! A9    A(2,3,4)             108.0            -DE/DX =    0.0                !
! A10   A(2,3,7)             125.967          -DE/DX =    0.0                !
! A11   A(4,3,7)             125.967          -DE/DX =    0.0                !
! A12   A(7,3,21)            125.3225         -DE/DX =    0.0                !
! A13   A(3,4,5)             108.0            -DE/DX =    0.0                !
! A14   A(3,4,8)             125.967          -DE/DX =    0.0                !
! A15   A(5,4,8)             125.967          -DE/DX =    0.0                !
! A16   A(8,4,21)            125.3225         -DE/DX =    0.0                !
! A17   A(1,5,4)             108.0            -DE/DX =    0.0                !
! A18   A(1,5,9)             125.967          -DE/DX =    0.0                !
! A19   A(4,5,9)             125.967          -DE/DX =    0.0                !
! A20   A(9,5,21)            125.3225         -DE/DX =    0.0                !
! A21   A(12,11,15)          108.0            -DE/DX =    0.0                !
! A22   A(12,11,16)          125.967          -DE/DX =    0.0                !
! A23   A(15,11,16)          125.967          -DE/DX =    0.0                !
! A24   A(16,11,21)          125.3225         -DE/DX =    0.0                !
! A25   A(11,12,13)          108.0            -DE/DX =    0.0                !
! A26   A(11,12,17)          125.967          -DE/DX =    0.0                !
! A27   A(13,12,17)          125.967          -DE/DX =    0.0                !
! A28   A(17,12,21)          125.3225         -DE/DX =    0.0                !
! A29   A(12,13,14)          108.0            -DE/DX =    0.0                !
! A30   A(12,13,18)          125.967          -DE/DX =    0.0                !
! A31   A(14,13,18)          125.967          -DE/DX =    0.0                !
! A32   A(18,13,21)          125.3225         -DE/DX =    0.0                !
! A33   A(13,14,15)          108.0            -DE/DX =    0.0                !
! A34   A(13,14,19)          125.967          -DE/DX =    0.0                !
! A35   A(15,14,19)          125.967          -DE/DX =    0.0                !
! A36   A(19,14,21)          125.3225         -DE/DX =    0.0                !
! A37   A(11,15,14)          108.0            -DE/DX =    0.0                !
! A38   A(11,15,20)          125.967          -DE/DX =    0.0                !
! A39   A(14,15,20)          125.967          -DE/DX =    0.0                !
! A40   A(20,15,21)          125.3225         -DE/DX =    0.0                !
! A41   A(1,21,3)             62.4674         -DE/DX =    0.0                !
! A42   A(1,21,4)             62.4674         -DE/DX =    0.0                !
! A43   A(1,21,11)           113.9213         -DE/DX =    0.0                !
! A44   A(1,21,12)           127.6534         -DE/DX =    0.0                !
! A45   A(1,21,13)           160.601          -DE/DX =    0.0                !
! A46   A(1,21,14)           160.601          -DE/DX =    0.0                !
! A47   A(1,21,15)           127.6534         -DE/DX =    0.0                !
! A48   A(2,21,4)             62.4674         -DE/DX =    0.0                !
! A49   A(2,21,5)             62.4674         -DE/DX =    0.0                !
! A50   A(2,21,11)           127.6534         -DE/DX =    0.0                !
! A51   A(2,21,12)           113.9213         -DE/DX =    0.0                !
! A52   A(2,21,13)           127.6534         -DE/DX =    0.0                !
! A53   A(2,21,14)           160.601          -DE/DX =    0.0                !
! A54   A(2,21,15)           160.601          -DE/DX =    0.0                !
! A55   A(3,21,5)             62.4674         -DE/DX =    0.0                !
! A56   A(3,21,11)           160.601          -DE/DX =    0.0                !
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! A57   A(3,21,12)          127.6534        -DE/DX =    0.0              !
! A58   A(3,21,13)          113.9213        -DE/DX =    0.0              !
! A59   A(3,21,14)          127.6534        -DE/DX =    0.0              !
! A60   A(3,21,15)          160.601         -DE/DX =    0.0              !
! A61   A(4,21,11)          160.601         -DE/DX =    0.0              !
! A62   A(4,21,12)          160.601         -DE/DX =    0.0              !
! A63   A(4,21,13)          127.6534        -DE/DX =    0.0              !
! A64   A(4,21,14)          113.9213        -DE/DX =    0.0              !
! A65   A(4,21,15)          127.6534        -DE/DX =    0.0              !
! A66   A(5,21,11)          127.6534        -DE/DX =    0.0              !
! A67   A(5,21,12)          160.601         -DE/DX =    0.0              !
! A68   A(5,21,13)          160.601         -DE/DX =    0.0              !
! A69   A(5,21,14)          127.6534        -DE/DX =    0.0              !
! A70   A(5,21,15)          113.9213        -DE/DX =    0.0              !
! A71   A(11,21,13)          62.4674        -DE/DX =    0.0              !
! A72   A(11,21,14)          62.4674        -DE/DX =    0.0              !
! A73   A(12,21,14)          62.4674        -DE/DX =    0.0              !
! A74   A(12,21,15)          62.4674        -DE/DX =    0.0              !
! A75   A(13,21,15)          62.4674        -DE/DX =    0.0              !
! D1    D(5,1,2,3)            0.0           -DE/DX =    0.0              !
! D2    D(5,1,2,6)         -177.1787        -DE/DX =    0.0              !
! D3    D(10,1,2,3)         177.1787        -DE/DX =    0.0              !
! D4    D(10,1,2,6)           0.0           -DE/DX =    0.0              !
! D5    D(2,1,5,4)            0.0           -DE/DX =    0.0              !
! D6    D(2,1,5,9)          177.1787        -DE/DX =    0.0              !
! D7    D(10,1,5,4)        -177.1787        -DE/DX =    0.0              !
! D8    D(10,1,5,9)           0.0           -DE/DX =    0.0              !
! D9    D(10,1,21,3)        158.8139        -DE/DX =    0.0              !
! D10   D(10,1,21,4)       -158.8139        -DE/DX =    0.0              !
! D11   D(10,1,21,11)          0.0           -DE/DX =    0.0              !
! D12   D(10,1,21,12)         40.9151        -DE/DX =    0.0              !
! D13   D(10,1,21,13)         74.7635        -DE/DX =    0.0              !
! D14   D(10,1,21,14)        -74.7635        -DE/DX =    0.0              !
! D15   D(10,1,21,15)        -40.9151        -DE/DX =    0.0              !
! D16   D(1,2,3,4)             0.0           -DE/DX =    0.0              !
! D17   D(1,2,3,7)          -177.1787        -DE/DX =    0.0              !
! D18   D(6,2,3,4)           177.1787        -DE/DX =    0.0              !
! D19   D(6,2,3,7)             0.0           -DE/DX =    0.0              !
! D20   D(6,2,21,4)          158.8139        -DE/DX =    0.0              !
! D21   D(6,2,21,5)         -158.8139        -DE/DX =    0.0              !
! D22   D(6,2,21,11)         -40.9151        -DE/DX =    0.0              !
! D23   D(6,2,21,12)           0.0           -DE/DX =    0.0              !
! D24   D(6,2,21,13)          40.9151        -DE/DX =    0.0              !
! D25   D(6,2,21,14)          74.7635        -DE/DX =    0.0              !
! D26   D(6,2,21,15)         -74.7635        -DE/DX =    0.0              !
! D27   D(2,3,4,5)             0.0           -DE/DX =    0.0              !
! D28   D(2,3,4,8)          -177.1787        -DE/DX =    0.0              !
! D29   D(7,3,4,5)           177.1787        -DE/DX =    0.0              !
! D30   D(7,3,4,8)             0.0           -DE/DX =    0.0              !
! D31   D(7,3,21,1)         -158.8139        -DE/DX =    0.0              !
```

```
! D32   D(7,3,21,5)          158.8139         -DE/DX =    0.0               !
! D33   D(7,3,21,11)         -74.7635         -DE/DX =    0.0               !
! D34   D(7,3,21,12)         -40.9151         -DE/DX =    0.0               !
! D35   D(7,3,21,13)           0.0            -DE/DX =    0.0               !
! D36   D(7,3,21,14)          40.9151         -DE/DX =    0.0               !
! D37   D(7,3,21,15)          74.7635         -DE/DX =    0.0               !
! D38   D(3,4,5,1)             0.0            -DE/DX =    0.0               !
! D39   D(3,4,5,9)          -177.1787         -DE/DX =    0.0               !
! D40   D(8,4,5,1)           177.1787         -DE/DX =    0.0               !
! D41   D(8,4,5,9)             0.0            -DE/DX =    0.0               !
! D42   D(8,4,21,1)          158.8139         -DE/DX =    0.0               !
! D43   D(8,4,21,2)         -158.8139         -DE/DX =    0.0               !
! D44   D(8,4,21,11)          74.7635         -DE/DX =    0.0               !
! D45   D(8,4,21,12)         -74.7635         -DE/DX =    0.0               !
! D46   D(8,4,21,13)         -40.9151         -DE/DX =    0.0               !
! D47   D(8,4,21,14)           0.0            -DE/DX =    0.0               !
! D48   D(8,4,21,15)          40.9151         -DE/DX =    0.0               !
! D49   D(9,5,21,2)          158.8139         -DE/DX =    0.0               !
! D50   D(9,5,21,3)         -158.8139         -DE/DX =    0.0               !
! D51   D(9,5,21,11)          40.9151         -DE/DX =    0.0               !
! D52   D(9,5,21,12)          74.7635         -DE/DX =    0.0               !
! D53   D(9,5,21,13)         -74.7635         -DE/DX =    0.0               !
! D54   D(9,5,21,14)         -40.9151         -DE/DX =    0.0               !
! D55   D(9,5,21,15)           0.0            -DE/DX =    0.0               !
! D56   D(15,11,12,13)         0.0            -DE/DX =    0.0               !
! D57   D(15,11,12,17)       177.1787         -DE/DX =    0.0               !
! D58   D(16,11,12,13)      -177.1787         -DE/DX =    0.0               !
! D59   D(16,11,12,17)         0.0            -DE/DX =    0.0               !
! D60   D(12,11,15,14)         0.0            -DE/DX =    0.0               !
! D61   D(12,11,15,20)      -177.1787         -DE/DX =    0.0               !
! D62   D(16,11,15,14)       177.1787         -DE/DX =    0.0               !
! D63   D(16,11,15,20)         0.0            -DE/DX =    0.0               !
! D64   D(16,11,21,1)          0.0            -DE/DX =    0.0               !
! D65   D(16,11,21,2)         -40.9151         -DE/DX =    0.0               !
! D66   D(16,11,21,3)         -74.7635         -DE/DX =    0.0               !
! D67   D(16,11,21,4)          74.7635         -DE/DX =    0.0               !
! D68   D(16,11,21,5)          40.9151         -DE/DX =    0.0               !
! D69   D(16,11,21,13)      -158.8139         -DE/DX =    0.0               !
! D70   D(16,11,21,14)       158.8139         -DE/DX =    0.0               !
! D71   D(11,12,13,14)         0.0            -DE/DX =    0.0               !
! D72   D(11,12,13,18)       177.1787         -DE/DX =    0.0               !
! D73   D(17,12,13,14)      -177.1787         -DE/DX =    0.0               !
! D74   D(17,12,13,18)         0.0            -DE/DX =    0.0               !
! D75   D(17,12,21,1)          40.9151         -DE/DX =    0.0               !
! D76   D(17,12,21,2)           0.0            -DE/DX =    0.0               !
! D77   D(17,12,21,3)         -40.9151         -DE/DX =    0.0               !
! D78   D(17,12,21,4)         -74.7635         -DE/DX =    0.0               !
! D79   D(17,12,21,5)          74.7635         -DE/DX =    0.0               !
! D80   D(17,12,21,14)      -158.8139         -DE/DX =    0.0               !
! D81   D(17,12,21,15)       158.8139         -DE/DX =    0.0               !
```

```
! D82   D(12,13,14,15)         0.0            -DE/DX =    0.0                 !
! D83   D(12,13,14,19)       177.1787         -DE/DX =    0.0                 !
! D84   D(18,13,14,15)      -177.1787         -DE/DX =    0.0                 !
! D85   D(18,13,14,19)         0.0            -DE/DX =    0.0                 !
! D86   D(18,13,21,1)         74.7635         -DE/DX =    0.0                 !
! D87   D(18,13,21,2)         40.9151         -DE/DX =    0.0                 !
! D88   D(18,13,21,3)          0.0            -DE/DX =    0.0                 !
! D89   D(18,13,21,4)        -40.9151         -DE/DX =    0.0                 !
! D90   D(18,13,21,5)        -74.7635         -DE/DX =    0.0                 !
! D91   D(18,13,21,11)       158.8139         -DE/DX =    0.0                 !
! D92   D(18,13,21,15)      -158.8139         -DE/DX =    0.0                 !
! D93   D(13,14,15,11)         0.0            -DE/DX =    0.0                 !
! D94   D(13,14,15,20)       177.1787         -DE/DX =    0.0                 !
! D95   D(19,14,15,11)      -177.1787         -DE/DX =    0.0                 !
! D96   D(19,14,15,20)         0.0            -DE/DX =    0.0                 !
! D97   D(19,14,21,1)        -74.7635         -DE/DX =    0.0                 !
! D98   D(19,14,21,2)         74.7635         -DE/DX =    0.0                 !
! D99   D(19,14,21,3)         40.9151         -DE/DX =    0.0                 !
! D100  D(19,14,21,4)          0.0            -DE/DX =    0.0                 !
! D101  D(19,14,21,5)        -40.9151         -DE/DX =    0.0                 !
! D102  D(19,14,21,11)      -158.8139         -DE/DX =    0.0                 !
! D103  D(19,14,21,12)       158.8139         -DE/DX =    0.0                 !
! D104  D(20,15,21,1)        -40.9151         -DE/DX =    0.0                 !
! D105  D(20,15,21,2)        -74.7635         -DE/DX =    0.0                 !
! D106  D(20,15,21,3)         74.7635         -DE/DX =    0.0                 !
! D107  D(20,15,21,4)         40.9151         -DE/DX =    0.0                 !
! D108  D(20,15,21,5)          0.0            -DE/DX =    0.0                 !
! D109  D(20,15,21,12)      -158.8139         -DE/DX =    0.0                 !
! D110  D(20,15,21,13)       158.8139         -DE/DX =    0.0                 !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1          6           0       -0.000000    1.224974   -1.883463
     2          6           0       -1.165019    0.378538   -1.883463
     3          6           0       -0.720022   -0.991025   -1.883463
     4          6           0        0.720022   -0.991025   -1.883463
     5          6           0        1.165019    0.378538   -1.883463
     6          1           0       -2.189806    0.711511   -1.926423
     7          1           0       -1.353374   -1.862760   -1.926423
     8          1           0        1.353374   -1.862760   -1.926423
     9          1           0        2.189806    0.711511   -1.926423
    10          1           0       -0.000000    2.302498   -1.926423
    11          6           0       -0.000000    1.224974    1.883463
    12          6           0       -1.165019    0.378538    1.883463
    13          6           0       -0.720022   -0.991025    1.883463
```

14	6	0	0.720022	-0.991025	1.883463
15	6	0	1.165019	0.378538	1.883463
16	1	0	-0.000000	2.302498	1.926423
17	1	0	-2.189806	0.711511	1.926423
18	1	0	-1.353374	-1.862760	1.926423
19	1	0	1.353374	-1.862760	1.926423
20	1	0	2.189806	0.711511	1.926423
21	44	0	-0.000000	0.000000	-0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.440043	0.000000			
3	C	2.330039	1.440043	0.000000		
4	C	2.330039	2.330039	1.440043	0.000000	
5	C	1.440043	2.330039	2.330039	1.440043	0.000000
6	H	2.249609	1.078380	2.249609	3.371582	3.371582
7	H	3.371582	2.249609	1.078380	2.249609	3.371582
8	H	3.371582	3.371582	2.249609	1.078380	2.249609
9	H	2.249609	3.371582	3.371582	2.249609	1.078380
10	H	1.078380	2.249609	3.371582	3.371582	2.249609
11	C	3.766925	4.032797	4.429312	4.429312	4.032797
12	C	4.032797	3.766925	4.032797	4.429312	4.429312
13	C	4.429312	4.032797	3.766925	4.032797	4.429312
14	C	4.429312	4.429312	4.032797	3.766925	4.032797
15	C	4.032797	4.429312	4.429312	4.032797	3.766925
16	H	3.959329	4.424265	5.087332	5.087332	4.424265
17	H	4.424265	3.959329	4.424265	5.087332	5.087332
18	H	5.087332	4.424265	3.959329	4.424265	5.087332
19	H	5.087332	5.087332	4.424265	3.959329	4.424265
20	H	4.424265	5.087332	5.087332	4.424265	3.959329
21	Ru	2.246774	2.246774	2.246774	2.246774	2.246774

		6	7	8	9	10
6	H	0.000000				
7	H	2.706749	0.000000			
8	H	4.379611	2.706749	0.000000		
9	H	4.379611	4.379611	2.706749	0.000000	
10	H	2.706749	4.379611	4.379611	2.706749	0.000000
11	C	4.424265	5.087332	5.087332	4.424265	3.959329
12	C	3.959329	4.424265	5.087332	5.087332	4.424265
13	C	4.424265	3.959329	4.424265	5.087332	5.087332
14	C	5.087332	4.424265	3.959329	4.424265	5.087332
15	C	5.087332	5.087332	4.424265	3.959329	4.424265
16	H	4.708600	5.833131	5.833131	4.708600	3.852846
17	H	3.852846	4.708600	5.833131	5.833131	4.708600
18	H	4.708600	3.852846	4.708600	5.833131	5.833131
19	H	5.833131	4.708600	3.852846	4.708600	5.833131
20	H	5.833131	5.833131	4.708600	3.852846	4.708600
21	Ru	3.002100	3.002100	3.002100	3.002100	3.002100

		11	12	13	14	15

```
   11  C    0.000000
   12  C    1.440043   0.000000
   13  C    2.330039   1.440043   0.000000
   14  C    2.330039   2.330039   1.440043   0.000000
   15  C    1.440043   2.330039   2.330039   1.440043   0.000000
   16  H    1.078380   2.249609   3.371582   3.371582   2.249609
   17  H    2.249609   1.078380   2.249609   3.371582   3.371582
   18  H    3.371582   2.249609   1.078380   2.249609   3.371582
   19  H    3.371582   3.371582   2.249609   1.078380   2.249609
   20  H    2.249609   3.371582   3.371582   2.249609   1.078380
   21  Ru   2.246774   2.246774   2.246774   2.246774   2.246774
                 16         17         18         19         20
   16  H    0.000000
   17  H    2.706749   0.000000
   18  H    4.379611   2.706749   0.000000
   19  H    4.379611   4.379611   2.706749   0.000000
   20  H    2.706749   4.379611   4.379611   2.706749   0.000000
   21  Ru   3.002100   3.002100   3.002100   3.002100   3.002100
                 21
   21  Ru   0.000000
Stoichiometry    C10H10Ru
Framework group  C1[X(C10H10Ru)]
Deg. of freedom    57
Prev. full point group           C1      NOp   1
Prev. largest Abelian subgroup   C1      NOp   1
      concise Abelian subgroup   C1      NOp   1
                  Standard orientation:
---------------------------------------------------------------------
Center     Atomic                     Coordinates (Angstroms)
Number     Number                        X           Y           Z
---------------------------------------------------------------------
     1          6                  -1.883463    1.224974    0.000003
     2          6                  -1.883463    0.378535    1.165020
     3          6                  -1.883463   -0.991026    0.720019
     4          6                  -1.883463   -0.991023   -0.720024
     5          6                  -1.883463    0.378540   -1.165019
     6          1                  -1.926423    0.711506    2.189807
     7          1                  -1.926423   -1.862763    1.353370
     8          1                  -1.926423   -1.862757   -1.353379
     9          1                  -1.926423    0.711516   -2.189804
    10          1                  -1.926423    2.302498    0.000005
    11          6                   1.883463    1.224974    0.000003
    12          6                   1.883463    0.378535    1.165020
    13          6                   1.883463   -0.991026    0.720019
    14          6                   1.883463   -0.991023   -0.720024
    15          6                   1.883463    0.378540   -1.165019
    16          1                   1.926423    2.302498    0.000005
    17          1                   1.926423    0.711506    2.189807
    18          1                   1.926423   -1.862763    1.353370
    19          1                   1.926423   -1.862757   -1.353379
```

```
     20          1                    1.926423    0.711516   -2.189804
     21         44                    0.000000    0.000000    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.1643904           0.8715809
0.8715809
 1\1\GINC-COMET-08-37\FOpt\RB3LYP\3-21G*\C10H10Ru1\GRIDCHEM\31-Jan-2021
 \0\\# opt=(calcfc,maxcycle=500) freq=noraman b3lyp/3-21g* symm=(follow
 ,pg=d5h)\\<Calculation as sent>\\0,1\C,0.,1.22497398,-1.88346255\C,-1.
 16501948,0.37853778,-1.88346255\C,-0.72002164,-0.99102476,-1.88346255\
 C,0.72002164,-0.99102476,-1.88346255\C,1.16501948,0.37853778,-1.883462
 55\H,-2.18980561,0.71151097,-1.926423\H,-1.35337429,-1.86275991,-1.926
 423\H,1.35337429,-1.86275991,-1.926423\H,2.18980561,0.71151097,-1.9264
 23\H,0.,2.30249788,-1.926423\C,0.,1.22497398,1.88346255\C,-1.16501948,
 0.37853778,1.88346255\C,-0.72002164,-0.99102476,1.88346255\C,0.7200216
 4,-0.99102476,1.88346255\C,1.16501948,0.37853778,1.88346255\H,0.,2.302
 49788,1.926423\H,-2.18980561,0.71151097,1.926423\H,-1.35337429,-1.8627
 5991,1.926423\H,1.35337429,-1.86275991,1.926423\H,2.18980561,0.7115109
 7,1.926423\Ru,0.,0.0000000029,0.\\Version=ES64L-G16RevB.01\State=1-A\H
 F=-4808.2057775\RMSD=8.957e-09\RMSF=4.876e-06\Dipole=0.,0.0000031,0.\P
 olar=0.,0.,0.,0.,0.,0.\Quadrupole=3.2038279,3.2036806,-6.4075085,0.,0.
 ,0.\PG=C01 [X(C10H10Ru1)]\\@


 VIRTUE IS LEARNED AT YOUR MOTHER'S KNEE,
 VICES ARE PICKED UP AT SOME OTHER JOINT.
 Job cpu time:       0 days  0 hours 14 minutes 53.9 seconds.
 Elapsed time:       0 days  0 hours  1 minutes  2.7 seconds.
 File lengths (MBytes):  RWF=     82 Int=      0 D2E=      0 Chk=      4 Scr=
1
 Normal termination of Gaussian 16 at Sun Jan 31 22:50:42 2021.
 Link1:  Proceeding to internal job step number  2.
 ----------------------------------------------------------------------
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/3-21G* Freq
 ----------------------------------------------------------------------
 1/6=500,10=4,29=7,30=1,38=1,40=1/1,3;
 2/12=2,40=1/2;
 3/5=5,7=1,11=2,14=-4,25=1,30=1,70=2,71=2,74=-5,116=1,140=1/1,2,3;
 4/5=101/1;
 5/5=2,38=6,98=1/2;
 8/6=4,10=90,11=11/1;
 11/6=1,8=1,9=11,15=111,16=1/1,2,10;
 10/6=1/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 7/8=1,10=1,25=1/1,2,3,16;
 1/6=500,10=4,30=1/3;
 99//99;
 Structure from the checkpoint file:
"/oasis/scratch/comet/gridchem/temp_project/38158479/Gau-23425.chk"
 ---------------------
 <Calculation as sent>
```

```
---------------------
Charge =  0 Multiplicity = 1
Redundant internal coordinates found in file.  (old form).
C,0,0.,1.22497398,-1.88346255
C,0,-1.16501948,0.37853778,-1.88346255
C,0,-0.72002164,-0.99102476,-1.88346255
C,0,0.72002164,-0.99102476,-1.88346255
C,0,1.16501948,0.37853778,-1.88346255
H,0,-2.18980561,0.71151097,-1.926423
H,0,-1.35337429,-1.86275991,-1.926423
H,0,1.35337429,-1.86275991,-1.926423
H,0,2.18980561,0.71151097,-1.926423
H,0,0.,2.30249788,-1.926423
C,0,0.,1.22497398,1.88346255
C,0,-1.16501948,0.37853778,1.88346255
C,0,-0.72002164,-0.99102476,1.88346255
C,0,0.72002164,-0.99102476,1.88346255
C,0,1.16501948,0.37853778,1.88346255
H,0,0.,2.30249788,1.926423
H,0,-2.18980561,0.71151097,1.926423
H,0,-1.35337429,-1.86275991,1.926423
H,0,1.35337429,-1.86275991,1.926423
H,0,2.18980561,0.71151097,1.926423
Ru,0,0.,0.0000000029,0.
Recover connectivity data from disk.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
--------------------------                            --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.44           calculate D2E/DX2 analytically  !
! R2    R(1,5)                  1.44           calculate D2E/DX2 analytically  !
! R3    R(1,10)                 1.0784         calculate D2E/DX2 analytically  !
! R4    R(1,21)                 2.2468         calculate D2E/DX2 analytically  !
! R5    R(2,3)                  1.44           calculate D2E/DX2 analytically  !
! R6    R(2,6)                  1.0784         calculate D2E/DX2 analytically  !
! R7    R(2,21)                 2.2468         calculate D2E/DX2 analytically  !
! R8    R(3,4)                  1.44           calculate D2E/DX2 analytically  !
! R9    R(3,7)                  1.0784         calculate D2E/DX2 analytically  !
! R10   R(3,21)                 2.2468         calculate D2E/DX2 analytically  !
! R11   R(4,5)                  1.44           calculate D2E/DX2 analytically  !
! R12   R(4,8)                  1.0784         calculate D2E/DX2 analytically  !
! R13   R(4,21)                 2.2468         calculate D2E/DX2 analytically  !
! R14   R(5,9)                  1.0784         calculate D2E/DX2 analytically  !
! R15   R(5,21)                 2.2468         calculate D2E/DX2 analytically  !
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! R16   R(11,12)              1.44          calculate D2E/DX2 analytically  !
! R17   R(11,15)              1.44          calculate D2E/DX2 analytically  !
! R18   R(11,16)              1.0784        calculate D2E/DX2 analytically  !
! R19   R(11,21)              2.2468        calculate D2E/DX2 analytically  !
! R20   R(12,13)              1.44          calculate D2E/DX2 analytically  !
! R21   R(12,17)              1.0784        calculate D2E/DX2 analytically  !
! R22   R(12,21)              2.2468        calculate D2E/DX2 analytically  !
! R23   R(13,14)              1.44          calculate D2E/DX2 analytically  !
! R24   R(13,18)              1.0784        calculate D2E/DX2 analytically  !
! R25   R(13,21)              2.2468        calculate D2E/DX2 analytically  !
! R26   R(14,15)              1.44          calculate D2E/DX2 analytically  !
! R27   R(14,19)              1.0784        calculate D2E/DX2 analytically  !
! R28   R(14,21)              2.2468        calculate D2E/DX2 analytically  !
! R29   R(15,20)              1.0784        calculate D2E/DX2 analytically  !
! R30   R(15,21)              2.2468        calculate D2E/DX2 analytically  !
! A1    A(2,1,5)            108.0           calculate D2E/DX2 analytically  !
! A2    A(2,1,10)           125.967         calculate D2E/DX2 analytically  !
! A3    A(5,1,10)           125.967         calculate D2E/DX2 analytically  !
! A4    A(10,1,21)          125.3225        calculate D2E/DX2 analytically  !
! A5    A(1,2,3)            108.0           calculate D2E/DX2 analytically  !
! A6    A(1,2,6)            125.967         calculate D2E/DX2 analytically  !
! A7    A(3,2,6)            125.967         calculate D2E/DX2 analytically  !
! A8    A(6,2,21)           125.3225        calculate D2E/DX2 analytically  !
! A9    A(2,3,4)            108.0           calculate D2E/DX2 analytically  !
! A10   A(2,3,7)            125.967         calculate D2E/DX2 analytically  !
! A11   A(4,3,7)            125.967         calculate D2E/DX2 analytically  !
! A12   A(7,3,21)           125.3225        calculate D2E/DX2 analytically  !
! A13   A(3,4,5)            108.0           calculate D2E/DX2 analytically  !
! A14   A(3,4,8)            125.967         calculate D2E/DX2 analytically  !
! A15   A(5,4,8)            125.967         calculate D2E/DX2 analytically  !
! A16   A(8,4,21)           125.3225        calculate D2E/DX2 analytically  !
! A17   A(1,5,4)            108.0           calculate D2E/DX2 analytically  !
! A18   A(1,5,9)            125.967         calculate D2E/DX2 analytically  !
! A19   A(4,5,9)            125.967         calculate D2E/DX2 analytically  !
! A20   A(9,5,21)           125.3225        calculate D2E/DX2 analytically  !
! A21   A(12,11,15)         108.0           calculate D2E/DX2 analytically  !
! A22   A(12,11,16)         125.967         calculate D2E/DX2 analytically  !
! A23   A(15,11,16)         125.967         calculate D2E/DX2 analytically  !
! A24   A(16,11,21)         125.3225        calculate D2E/DX2 analytically  !
! A25   A(11,12,13)         108.0           calculate D2E/DX2 analytically  !
! A26   A(11,12,17)         125.967         calculate D2E/DX2 analytically  !
! A27   A(13,12,17)         125.967         calculate D2E/DX2 analytically  !
! A28   A(17,12,21)         125.3225        calculate D2E/DX2 analytically  !
! A29   A(12,13,14)         108.0           calculate D2E/DX2 analytically  !
! A30   A(12,13,18)         125.967         calculate D2E/DX2 analytically  !
! A31   A(14,13,18)         125.967         calculate D2E/DX2 analytically  !
! A32   A(18,13,21)         125.3225        calculate D2E/DX2 analytically  !
! A33   A(13,14,15)         108.0           calculate D2E/DX2 analytically  !
! A34   A(13,14,19)         125.967         calculate D2E/DX2 analytically  !
! A35   A(15,14,19)         125.967         calculate D2E/DX2 analytically  !
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! A36   A(19,14,21)          125.3225         calculate D2E/DX2 analytically  !
! A37   A(11,15,14)          108.0            calculate D2E/DX2 analytically  !
! A38   A(11,15,20)          125.967          calculate D2E/DX2 analytically  !
! A39   A(14,15,20)          125.967          calculate D2E/DX2 analytically  !
! A40   A(20,15,21)          125.3225         calculate D2E/DX2 analytically  !
! A41   A(1,21,3)             62.4674         calculate D2E/DX2 analytically  !
! A42   A(1,21,4)             62.4674         calculate D2E/DX2 analytically  !
! A43   A(1,21,11)           113.9213         calculate D2E/DX2 analytically  !
! A44   A(1,21,12)           127.6534         calculate D2E/DX2 analytically  !
! A45   A(1,21,13)           160.601          calculate D2E/DX2 analytically  !
! A46   A(1,21,14)           160.601          calculate D2E/DX2 analytically  !
! A47   A(1,21,15)           127.6534         calculate D2E/DX2 analytically  !
! A48   A(2,21,4)             62.4674         calculate D2E/DX2 analytically  !
! A49   A(2,21,5)             62.4674         calculate D2E/DX2 analytically  !
! A50   A(2,21,11)           127.6534         calculate D2E/DX2 analytically  !
! A51   A(2,21,12)           113.9213         calculate D2E/DX2 analytically  !
! A52   A(2,21,13)           127.6534         calculate D2E/DX2 analytically  !
! A53   A(2,21,14)           160.601          calculate D2E/DX2 analytically  !
! A54   A(2,21,15)           160.601          calculate D2E/DX2 analytically  !
! A55   A(3,21,5)             62.4674         calculate D2E/DX2 analytically  !
! A56   A(3,21,11)           160.601          calculate D2E/DX2 analytically  !
! A57   A(3,21,12)           127.6534         calculate D2E/DX2 analytically  !
! A58   A(3,21,13)           113.9213         calculate D2E/DX2 analytically  !
! A59   A(3,21,14)           127.6534         calculate D2E/DX2 analytically  !
! A60   A(3,21,15)           160.601          calculate D2E/DX2 analytically  !
! A61   A(4,21,11)           160.601          calculate D2E/DX2 analytically  !
! A62   A(4,21,12)           160.601          calculate D2E/DX2 analytically  !
! A63   A(4,21,13)           127.6534         calculate D2E/DX2 analytically  !
! A64   A(4,21,14)           113.9213         calculate D2E/DX2 analytically  !
! A65   A(4,21,15)           127.6534         calculate D2E/DX2 analytically  !
! A66   A(5,21,11)           127.6534         calculate D2E/DX2 analytically  !
! A67   A(5,21,12)           160.601          calculate D2E/DX2 analytically  !
! A68   A(5,21,13)           160.601          calculate D2E/DX2 analytically  !
! A69   A(5,21,14)           127.6534         calculate D2E/DX2 analytically  !
! A70   A(5,21,15)           113.9213         calculate D2E/DX2 analytically  !
! A71   A(11,21,13)           62.4674         calculate D2E/DX2 analytically  !
! A72   A(11,21,14)           62.4674         calculate D2E/DX2 analytically  !
! A73   A(12,21,14)           62.4674         calculate D2E/DX2 analytically  !
! A74   A(12,21,15)           62.4674         calculate D2E/DX2 analytically  !
! A75   A(13,21,15)           62.4674         calculate D2E/DX2 analytically  !
! D1    D(5,1,2,3)             0.0            calculate D2E/DX2 analytically  !
! D2    D(5,1,2,6)          -177.1787         calculate D2E/DX2 analytically  !
! D3    D(10,1,2,3)          177.1787         calculate D2E/DX2 analytically  !
! D4    D(10,1,2,6)            0.0            calculate D2E/DX2 analytically  !
! D5    D(2,1,5,4)             0.0            calculate D2E/DX2 analytically  !
! D6    D(2,1,5,9)           177.1787         calculate D2E/DX2 analytically  !
! D7    D(10,1,5,4)         -177.1787         calculate D2E/DX2 analytically  !
! D8    D(10,1,5,9)            0.0            calculate D2E/DX2 analytically  !
! D9    D(10,1,21,3)         158.8139         calculate D2E/DX2 analytically  !
! D10   D(10,1,21,4)        -158.8139         calculate D2E/DX2 analytically  !
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! D11   D(10,1,21,11)          0.0           calculate D2E/DX2 analytically  !
! D12   D(10,1,21,12)         40.9151        calculate D2E/DX2 analytically  !
! D13   D(10,1,21,13)         74.7635        calculate D2E/DX2 analytically  !
! D14   D(10,1,21,14)        -74.7635        calculate D2E/DX2 analytically  !
! D15   D(10,1,21,15)        -40.9151        calculate D2E/DX2 analytically  !
! D16   D(1,2,3,4)             0.0           calculate D2E/DX2 analytically  !
! D17   D(1,2,3,7)          -177.1787        calculate D2E/DX2 analytically  !
! D18   D(6,2,3,4)           177.1787        calculate D2E/DX2 analytically  !
! D19   D(6,2,3,7)             0.0           calculate D2E/DX2 analytically  !
! D20   D(6,2,21,4)          158.8139        calculate D2E/DX2 analytically  !
! D21   D(6,2,21,5)         -158.8139        calculate D2E/DX2 analytically  !
! D22   D(6,2,21,11)         -40.9151        calculate D2E/DX2 analytically  !
! D23   D(6,2,21,12)           0.0           calculate D2E/DX2 analytically  !
! D24   D(6,2,21,13)          40.9151        calculate D2E/DX2 analytically  !
! D25   D(6,2,21,14)          74.7635        calculate D2E/DX2 analytically  !
! D26   D(6,2,21,15)         -74.7635        calculate D2E/DX2 analytically  !
! D27   D(2,3,4,5)             0.0           calculate D2E/DX2 analytically  !
! D28   D(2,3,4,8)          -177.1787        calculate D2E/DX2 analytically  !
! D29   D(7,3,4,5)           177.1787        calculate D2E/DX2 analytically  !
! D30   D(7,3,4,8)             0.0           calculate D2E/DX2 analytically  !
! D31   D(7,3,21,1)         -158.8139        calculate D2E/DX2 analytically  !
! D32   D(7,3,21,5)          158.8139        calculate D2E/DX2 analytically  !
! D33   D(7,3,21,11)         -74.7635        calculate D2E/DX2 analytically  !
! D34   D(7,3,21,12)         -40.9151        calculate D2E/DX2 analytically  !
! D35   D(7,3,21,13)           0.0           calculate D2E/DX2 analytically  !
! D36   D(7,3,21,14)          40.9151        calculate D2E/DX2 analytically  !
! D37   D(7,3,21,15)          74.7635        calculate D2E/DX2 analytically  !
! D38   D(3,4,5,1)             0.0           calculate D2E/DX2 analytically  !
! D39   D(3,4,5,9)          -177.1787        calculate D2E/DX2 analytically  !
! D40   D(8,4,5,1)           177.1787        calculate D2E/DX2 analytically  !
! D41   D(8,4,5,9)             0.0           calculate D2E/DX2 analytically  !
! D42   D(8,4,21,1)          158.8139        calculate D2E/DX2 analytically  !
! D43   D(8,4,21,2)         -158.8139        calculate D2E/DX2 analytically  !
! D44   D(8,4,21,11)          74.7635        calculate D2E/DX2 analytically  !
! D45   D(8,4,21,12)         -74.7635        calculate D2E/DX2 analytically  !
! D46   D(8,4,21,13)         -40.9151        calculate D2E/DX2 analytically  !
! D47   D(8,4,21,14)           0.0           calculate D2E/DX2 analytically  !
! D48   D(8,4,21,15)          40.9151        calculate D2E/DX2 analytically  !
! D49   D(9,5,21,2)          158.8139        calculate D2E/DX2 analytically  !
! D50   D(9,5,21,3)         -158.8139        calculate D2E/DX2 analytically  !
! D51   D(9,5,21,11)          40.9151        calculate D2E/DX2 analytically  !
! D52   D(9,5,21,12)          74.7635        calculate D2E/DX2 analytically  !
! D53   D(9,5,21,13)         -74.7635        calculate D2E/DX2 analytically  !
! D54   D(9,5,21,14)         -40.9151        calculate D2E/DX2 analytically  !
! D55   D(9,5,21,15)           0.0           calculate D2E/DX2 analytically  !
! D56   D(15,11,12,13)         0.0           calculate D2E/DX2 analytically  !
! D57   D(15,11,12,17)       177.1787        calculate D2E/DX2 analytically  !
! D58   D(16,11,12,13)      -177.1787        calculate D2E/DX2 analytically  !
! D59   D(16,11,12,17)         0.0           calculate D2E/DX2 analytically  !
! D60   D(12,11,15,14)         0.0           calculate D2E/DX2 analytically  !
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! D61   D(12,11,15,20)      -177.1787        calculate D2E/DX2 analytically  !
! D62   D(16,11,15,14)       177.1787        calculate D2E/DX2 analytically  !
! D63   D(16,11,15,20)         0.0           calculate D2E/DX2 analytically  !
! D64   D(16,11,21,1)          0.0           calculate D2E/DX2 analytically  !
! D65   D(16,11,21,2)        -40.9151        calculate D2E/DX2 analytically  !
! D66   D(16,11,21,3)        -74.7635        calculate D2E/DX2 analytically  !
! D67   D(16,11,21,4)         74.7635        calculate D2E/DX2 analytically  !
! D68   D(16,11,21,5)         40.9151        calculate D2E/DX2 analytically  !
! D69   D(16,11,21,13)      -158.8139        calculate D2E/DX2 analytically  !
! D70   D(16,11,21,14)       158.8139        calculate D2E/DX2 analytically  !
! D71   D(11,12,13,14)         0.0           calculate D2E/DX2 analytically  !
! D72   D(11,12,13,18)       177.1787        calculate D2E/DX2 analytically  !
! D73   D(17,12,13,14)      -177.1787        calculate D2E/DX2 analytically  !
! D74   D(17,12,13,18)         0.0           calculate D2E/DX2 analytically  !
! D75   D(17,12,21,1)         40.9151        calculate D2E/DX2 analytically  !
! D76   D(17,12,21,2)          0.0           calculate D2E/DX2 analytically  !
! D77   D(17,12,21,3)        -40.9151        calculate D2E/DX2 analytically  !
! D78   D(17,12,21,4)        -74.7635        calculate D2E/DX2 analytically  !
! D79   D(17,12,21,5)         74.7635        calculate D2E/DX2 analytically  !
! D80   D(17,12,21,14)      -158.8139        calculate D2E/DX2 analytically  !
! D81   D(17,12,21,15)       158.8139        calculate D2E/DX2 analytically  !
! D82   D(12,13,14,15)         0.0           calculate D2E/DX2 analytically  !
! D83   D(12,13,14,19)       177.1787        calculate D2E/DX2 analytically  !
! D84   D(18,13,14,15)      -177.1787        calculate D2E/DX2 analytically  !
! D85   D(18,13,14,19)         0.0           calculate D2E/DX2 analytically  !
! D86   D(18,13,21,1)         74.7635        calculate D2E/DX2 analytically  !
! D87   D(18,13,21,2)         40.9151        calculate D2E/DX2 analytically  !
! D88   D(18,13,21,3)          0.0           calculate D2E/DX2 analytically  !
! D89   D(18,13,21,4)        -40.9151        calculate D2E/DX2 analytically  !
! D90   D(18,13,21,5)        -74.7635        calculate D2E/DX2 analytically  !
! D91   D(18,13,21,11)       158.8139        calculate D2E/DX2 analytically  !
! D92   D(18,13,21,15)      -158.8139        calculate D2E/DX2 analytically  !
! D93   D(13,14,15,11)         0.0           calculate D2E/DX2 analytically  !
! D94   D(13,14,15,20)       177.1787        calculate D2E/DX2 analytically  !
! D95   D(19,14,15,11)      -177.1787        calculate D2E/DX2 analytically  !
! D96   D(19,14,15,20)         0.0           calculate D2E/DX2 analytically  !
! D97   D(19,14,21,1)        -74.7635        calculate D2E/DX2 analytically  !
! D98   D(19,14,21,2)         74.7635        calculate D2E/DX2 analytically  !
! D99   D(19,14,21,3)         40.9151        calculate D2E/DX2 analytically  !
! D100  D(19,14,21,4)          0.0           calculate D2E/DX2 analytically  !
! D101  D(19,14,21,5)        -40.9151        calculate D2E/DX2 analytically  !
! D102  D(19,14,21,11)      -158.8139        calculate D2E/DX2 analytically  !
! D103  D(19,14,21,12)       158.8139        calculate D2E/DX2 analytically  !
! D104  D(20,15,21,1)        -40.9151        calculate D2E/DX2 analytically  !
! D105  D(20,15,21,2)        -74.7635        calculate D2E/DX2 analytically  !
! D106  D(20,15,21,3)         74.7635        calculate D2E/DX2 analytically  !
! D107  D(20,15,21,4)         40.9151        calculate D2E/DX2 analytically  !
! D108  D(20,15,21,5)          0.0           calculate D2E/DX2 analytically  !
! D109  D(20,15,21,12)      -158.8139        calculate D2E/DX2 analytically  !
! D110  D(20,15,21,13)       158.8139        calculate D2E/DX2 analytically  !
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 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07 EigMax=2.50D+02
EigMin=1.00D-04
 Number of steps in this run=      2 maximum allowed number of steps=      2.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -0.000000    1.224974   -1.883463
      2          6           0       -1.165019    0.378538   -1.883463
      3          6           0       -0.720022   -0.991025   -1.883463
      4          6           0        0.720022   -0.991025   -1.883463
      5          6           0        1.165019    0.378538   -1.883463
      6          1           0       -2.189806    0.711511   -1.926423
      7          1           0       -1.353374   -1.862760   -1.926423
      8          1           0        1.353374   -1.862760   -1.926423
      9          1           0        2.189806    0.711511   -1.926423
     10          1           0       -0.000000    2.302498   -1.926423
     11          6           0       -0.000000    1.224974    1.883463
     12          6           0       -1.165019    0.378538    1.883463
     13          6           0       -0.720022   -0.991025    1.883463
     14          6           0        0.720022   -0.991025    1.883463
     15          6           0        1.165019    0.378538    1.883463
     16          1           0       -0.000000    2.302498    1.926423
     17          1           0       -2.189806    0.711511    1.926423
     18          1           0       -1.353374   -1.862760    1.926423
     19          1           0        1.353374   -1.862760    1.926423
     20          1           0        2.189806    0.711511    1.926423
     21         44           0        0.000000    0.000000   -0.000000
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                      1          2          3          4          5
    1  C    0.000000
    2  C    1.440043   0.000000
    3  C    2.330039   1.440043   0.000000
    4  C    2.330039   2.330039   1.440043   0.000000
    5  C    1.440043   2.330039   2.330039   1.440043   0.000000
    6  H    2.249609   1.078380   2.249609   3.371582   3.371582
    7  H    3.371582   2.249609   1.078380   2.249609   3.371582
    8  H    3.371582   3.371582   2.249609   1.078380   2.249609
    9  H    2.249609   3.371582   3.371582   2.249609   1.078380
   10  H    1.078380   2.249609   3.371582   3.371582   2.249609
   11  C    3.766925   4.032797   4.429312   4.429312   4.032797
   12  C    4.032797   3.766925   4.032797   4.429312   4.429312
   13  C    4.429312   4.032797   3.766925   4.032797   4.429312
   14  C    4.429312   4.429312   4.032797   3.766925   4.032797
   15  C    4.032797   4.429312   4.429312   4.032797   3.766925
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16	H	3.959329	4.424265	5.087332	5.087332	4.424265
17	H	4.424265	3.959329	4.424265	5.087332	5.087332
18	H	5.087332	4.424265	3.959329	4.424265	5.087332
19	H	5.087332	5.087332	4.424265	3.959329	4.424265
20	H	4.424265	5.087332	5.087332	4.424265	3.959329
21	Ru	2.246774	2.246774	2.246774	2.246774	2.246774

		6	7	8	9	10
6	H	0.000000				
7	H	2.706749	0.000000			
8	H	4.379611	2.706749	0.000000		
9	H	4.379611	4.379611	2.706749	0.000000	
10	H	2.706749	4.379611	4.379611	2.706749	0.000000
11	C	4.424265	5.087332	5.087332	4.424265	3.959329
12	C	3.959329	4.424265	5.087332	5.087332	4.424265
13	C	4.424265	3.959329	4.424265	5.087332	5.087332
14	C	5.087332	4.424265	3.959329	4.424265	5.087332
15	C	5.087332	5.087332	4.424265	3.959329	4.424265
16	H	4.708600	5.833131	5.833131	4.708600	3.852846
17	H	3.852846	4.708600	5.833131	5.833131	4.708600
18	H	4.708600	3.852846	4.708600	5.833131	5.833131
19	H	5.833131	4.708600	3.852846	4.708600	5.833131
20	H	5.833131	5.833131	4.708600	3.852846	4.708600
21	Ru	3.002100	3.002100	3.002100	3.002100	3.002100

		11	12	13	14	15
11	C	0.000000				
12	C	1.440043	0.000000			
13	C	2.330039	1.440043	0.000000		
14	C	2.330039	2.330039	1.440043	0.000000	
15	C	1.440043	2.330039	2.330039	1.440043	0.000000
16	H	1.078380	2.249609	3.371582	3.371582	2.249609
17	H	2.249609	1.078380	2.249609	3.371582	3.371582
18	H	3.371582	2.249609	1.078380	2.249609	3.371582
19	H	3.371582	3.371582	2.249609	1.078380	2.249609
20	H	2.249609	3.371582	3.371582	2.249609	1.078380
21	Ru	2.246774	2.246774	2.246774	2.246774	2.246774

		16	17	18	19	20
16	H	0.000000				
17	H	2.706749	0.000000			
18	H	4.379611	2.706749	0.000000		
19	H	4.379611	4.379611	2.706749	0.000000	
20	H	2.706749	4.379611	4.379611	2.706749	0.000000
21	Ru	3.002100	3.002100	3.002100	3.002100	3.002100

		21
21	Ru	0.000000

Stoichiometry C10H10Ru
Framework group D5H[O(Ru),5SGV(C2H2)]
Deg. of freedom 4
Full point group D5H NOp 20
Largest Abelian subgroup C2V NOp 4
Largest concise Abelian subgroup C2V NOp 4

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        0.000000    1.224974    1.883463
      2          6           0        1.165019    0.378538    1.883463
      3          6           0        0.720022   -0.991025    1.883463
      4          6           0       -0.720022   -0.991025    1.883463
      5          6           0       -1.165019    0.378538    1.883463
      6          1           0        2.189806    0.711511    1.926423
      7          1           0        1.353374   -1.862760    1.926423
      8          1           0       -1.353374   -1.862760    1.926423
      9          1           0       -2.189806    0.711511    1.926423
     10          1           0        0.000000    2.302498    1.926423
     11          6           0        0.000000    1.224974   -1.883463
     12          6           0        1.165019    0.378538   -1.883463
     13          6           0        0.720022   -0.991025   -1.883463
     14          6           0       -0.720022   -0.991025   -1.883463
     15          6           0       -1.165019    0.378538   -1.883463
     16          1           0       -0.000000    2.302498   -1.926423
     17          1           0        2.189806    0.711511   -1.926423
     18          1           0        1.353374   -1.862760   -1.926423
     19          1           0       -1.353374   -1.862760   -1.926423
     20          1           0       -2.189806    0.711511   -1.926423
     21         44           0        0.000000    0.000000    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.1643904           0.8715809
0.8715809
 Standard basis: 3-21G* (6D, 7F)
 There are    51 symmetry adapted cartesian basis functions of A1  symmetry.
 There are    27 symmetry adapted cartesian basis functions of A2  symmetry.
 There are    32 symmetry adapted cartesian basis functions of B1  symmetry.
 There are    39 symmetry adapted cartesian basis functions of B2  symmetry.
 There are    51 symmetry adapted basis functions of A1  symmetry.
 There are    27 symmetry adapted basis functions of A2  symmetry.
 There are    32 symmetry adapted basis functions of B1  symmetry.
 There are    39 symmetry adapted basis functions of B2  symmetry.
   149 basis functions,   267 primitive gaussians,   149 cartesian basis functions
    57 alpha electrons       57 beta electrons
       nuclear repulsion energy      1146.1765806597 Hartrees.
 NAtoms=   21 NActive=   21 NUniq=    3 SFac= 4.00D+00 NAtFMM=   60 NAOKFM=F Big=F
 Integral buffers will be    131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=   149 RedAO= T EigKep=  1.33D-03  NBF=    51    27    32    39
 NBsUse=   149 1.00D-06 EigRej= -1.00D+00 NBFU=    51    27    32    39
 Defaulting to unpruned grid for atomic number  44.
 Initial guess from the checkpoint file:
```

```
"/oasis/scratch/comet/gridchem/temp_project/38158479/Gau-23425.chk"
 B after Tr=    -0.000000   -0.000000    0.000000
         Rot=    0.707107    0.000000   -0.707107   -0.000000 Ang=  90.00 deg.
 Initial guess orbital symmetries:
       Occupied  (A1') (A1') (A2") (E1') (E1') (A1') (A2") (E1')
                 (E1') (A1') (E1") (E1") (E2') (E2') (E2') (E2')
                 (E2") (E2") (A2") (E1") (E1") (E1') (E1') (A1')
                 (A1') (A2") (E1') (E1') (A1') (A2") (E1") (E1")
                 (E1') (E1') (E2') (E2') (E2") (E2") (A1') (A2")
                 (E1") (E1") (E1') (E1') (A1') (E2') (E2') (E2")
                 (E2") (A2") (E1") (E1") (E1') (E1') (A1') (E2')
                 (E2')
       Virtual   (E1") (E1") (A1') (E1') (E1') (A2") (E2") (E2")
                 (E2') (E2') (A2") (A1') (E2') (E2') (E2") (E2")
                 (E1") (E1") (E1') (E1') (E1') (E1') (E1") (E1")
                 (A1') (E1') (E1') (E2') (E2') (E2") (E2") (A2')
                 (A1") (A1') (A2") (E2') (E2') (E1") (E1") (E2")
                 (E2") (A1') (A2") (E1') (E1') (E2') (E2') (E1")
                 (E1") (A1') (E2") (E2") (A2") (E1') (E1') (E2')
                 (E2') (E2") (E2") (A2') (A1") (E1") (E1") (E1')
                 (E1') (A2") (A1') (E2') (E2') (E1") (E1") (E1')
                 (E1') (A1') (E2') (E2') (E1") (E1") (E2") (E2")
                 (A1') (E1') (E1') (E2") (E2") (A2") (E1") (E1")
                 (E2') (E2') (A1') (A1')
 Keep R1 ints in memory in symmetry-blocked form, NReq=78136020.
 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.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
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 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 SCF Done:  E(RB3LYP) =  -4808.20578387     A.U. after    5 cycles
            NFock=  5  Conv=0.48D-08     -V/T= 2.0049
 DoSCS=F DFT=T ScalE2(SS,OS)=  1.000000  1.000000
 Range of M.O.s used for correlation:     1   149
 NBasis=   149 NAE=    57 NBE=    57 NFC=     0 NFV=     0
```

```
NROrb=    149 NOA=    57 NOB=    57 NVA=    92 NVB=    92

**** Warning!!: The largest alpha MO coefficient is  0.20105565D+02

Symmetrizing basis deriv contribution to polar:
IMax=3 JMax=2 DiffMx= 0.00D+00
G2DrvN: will do    22 centers at a time, making    1 passes.
Calling FoFCou, ICntrl=  3107 FMM=F I1Cent=   0 AccDes= 0.00D+00.
Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
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Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
End of G2Drv F.D. properties file   721 does not exist.
End of G2Drv F.D. properties file   722 does not exist.
End of G2Drv F.D. properties file   788 does not exist.
         IDoAtm=11111111111111111111
         Differentiating once with respect to electric field.
               with respect to dipole field.
         Differentiating once with respect to nuclear coordinates.
Defaulting to unpruned grid for atomic number  44.
Keep R1 ints in memory in symmetry-blocked form, NReq=78145282.
Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
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Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
Defaulting to unpruned grid for atomic number  44.
         There are    12 degrees of freedom in the 1st order CPHF.  IDoFFX=4
```

```
NUNeed=    12.
     12 vectors produced by pass  0 Test12= 4.37D-14 8.33D-09 XBig12= 2.43D+02
9.08D+00.
 AX will form    12 AO Fock derivatives at one time.
     12 vectors produced by pass  1 Test12= 4.37D-14 8.33D-09 XBig12= 5.53D+01
2.06D+00.
     12 vectors produced by pass  2 Test12= 4.37D-14 8.33D-09 XBig12= 2.47D+00
3.24D-01.
     12 vectors produced by pass  3 Test12= 4.37D-14 8.33D-09 XBig12= 1.32D-02
3.16D-02.
     12 vectors produced by pass  4 Test12= 4.37D-14 8.33D-09 XBig12= 1.30D-04
4.15D-03.
     12 vectors produced by pass  5 Test12= 4.37D-14 8.33D-09 XBig12= 3.96D-06
5.57D-04.
     12 vectors produced by pass  6 Test12= 4.37D-14 8.33D-09 XBig12= 1.21D-07
7.76D-05.
      9 vectors produced by pass  7 Test12= 4.37D-14 8.33D-09 XBig12= 1.60D-09
9.09D-06.
      8 vectors produced by pass  8 Test12= 4.37D-14 8.33D-09 XBig12= 1.23D-11
6.49D-07.
      3 vectors produced by pass  9 Test12= 4.37D-14 8.33D-09 XBig12= 8.26D-14
5.18D-08.
 InvSVY:  IOpt=1 It=  1 EMax= 3.55D-15
 Solved reduced A of dimension   104 with    12 vectors.
 Isotropic polarizability for W=    0.000000      115.05 Bohr**3.
 End of Minotr F.D. properties file   721 does not exist.
 End of Minotr F.D. properties file   722 does not exist.
 End of Minotr F.D. properties file   788 does not exist.

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

           Population analysis using the SCF Density.

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

 Orbital symmetries:
       Occupied  (A1') (A1') (A2") (E1') (E1') (A1') (A2") (E1')
                 (E1') (A1') (E1") (E1") (E2') (E2') (E2') (E2')
                 (E2") (E2") (A2") (E1") (E1") (E1') (E1') (A1')
                 (A1') (A2") (E1') (E1') (A1') (A2") (E1") (E1")
                 (E1') (E1') (E2') (E2') (E2") (E2") (A1') (A2")
                 (E1") (E1") (E1') (E1') (A1') (E2') (E2') (E2")
                 (E2") (A2") (E1") (E1") (E1') (E1') (A1') (E2')
                 (E2')
       Virtual   (E1") (E1") (A1') (E1') (E1') (A2") (E2") (E2")
                 (E2') (E2') (A2") (A1') (E2') (E2') (E2") (E2")
                 (E1") (E1") (E1') (E1') (E1') (E1') (E1") (E1")
                 (A1') (E1') (E1') (E2') (E2') (E2") (E2") (A2')
                 (A1") (A1') (A2") (E2') (E2') (E1") (E1") (E2")
                 (E2") (A1') (A2") (E1') (E1') (E2') (E2') (E1")
```

```
               (E1") (A1') (E2") (E2") (A2") (E1') (E1') (E2')
               (E2') (E2") (E2") (A2') (A1") (E1") (E1") (E1')
               (E1') (A2") (A1') (E2') (E2') (E1") (E1") (E1')
               (E1') (A1') (E2') (E2') (E1") (E1") (E2") (E2")
               (A1') (E1') (E1') (E2") (E2") (A2") (E1") (E1")
               (E2') (E2') (A1') (A1')
The electronic state is 1-A1'.
Alpha  occ. eigenvalues -- -781.88987-111.30451-102.62951-102.62282-102.62282
Alpha  occ. eigenvalues --  -19.87367 -16.30147 -16.28637 -16.28637 -10.49043
Alpha  occ. eigenvalues --  -10.48816 -10.48816 -10.47830 -10.47830 -10.13575
Alpha  occ. eigenvalues --  -10.13575 -10.13545 -10.13545 -10.13541 -10.13539
Alpha  occ. eigenvalues --  -10.13539 -10.13516 -10.13516 -10.13454  -2.74356
Alpha  occ. eigenvalues --   -1.69701  -1.64619  -1.64619  -0.88958  -0.87264
Alpha  occ. eigenvalues --   -0.71486  -0.71486  -0.70845  -0.70845  -0.54673
Alpha  occ. eigenvalues --   -0.54673  -0.54239  -0.54239  -0.53731  -0.52612
Alpha  occ. eigenvalues --   -0.41576  -0.41576  -0.40439  -0.40439  -0.40056
Alpha  occ. eigenvalues --   -0.38171  -0.38171  -0.37957  -0.37957  -0.35490
Alpha  occ. eigenvalues --   -0.28656  -0.28656  -0.23020  -0.23020  -0.21002
Alpha  occ. eigenvalues --   -0.19397  -0.19397
Alpha virt. eigenvalues --   -0.00195  -0.00195   0.02672   0.03551   0.03551
Alpha virt. eigenvalues --    0.05362   0.05965   0.05965   0.08746   0.08746
Alpha virt. eigenvalues --    0.16813   0.17438   0.18616   0.18616   0.19402
Alpha virt. eigenvalues --    0.19402   0.19553   0.19553   0.20372   0.20372
Alpha virt. eigenvalues --    0.24683   0.24683   0.25190   0.25190   0.25892
Alpha virt. eigenvalues --    0.31000   0.31000   0.39011   0.39011   0.39608
Alpha virt. eigenvalues --    0.39608   0.44259   0.44600   0.44879   0.50271
Alpha virt. eigenvalues --    0.69657   0.69657   0.71633   0.71633   0.71714
Alpha virt. eigenvalues --    0.71714   0.76760   0.77130   0.77832   0.77832
Alpha virt. eigenvalues --    0.79768   0.79768   0.83880   0.83880   0.86477
Alpha virt. eigenvalues --    0.88184   0.88184   0.91362   0.96775   0.96775
Alpha virt. eigenvalues --    0.98174   0.98174   0.98757   0.98757   1.00969
Alpha virt. eigenvalues --    1.01999   1.05437   1.05437   1.10319   1.10319
Alpha virt. eigenvalues --    1.17720   1.19752   1.20216   1.20216   1.26160
Alpha virt. eigenvalues --    1.26160   1.34726   1.34726   1.36731   1.37604
Alpha virt. eigenvalues --    1.37604   1.38899   1.38899   1.39618   1.39618
Alpha virt. eigenvalues --    1.93555   2.00504   2.00504   2.02444   2.02444
Alpha virt. eigenvalues --    2.28875   2.42659   2.42659   2.43733   2.43733
Alpha virt. eigenvalues --    3.24387 152.27236
          Condensed to atoms (all electrons):
               1         2         3         4         5         6
     1  C    5.473619  0.360190 -0.118533 -0.118533  0.360190 -0.028544
     2  C    0.360190  5.473619  0.360190 -0.118533 -0.118533  0.399486
     3  C   -0.118533  0.360190  5.473619  0.360190 -0.118533 -0.028544
     4  C   -0.118533 -0.118533  0.360190  5.473619  0.360190  0.003143
     5  C    0.360190 -0.118533 -0.118533  0.360190  5.473619  0.003143
     6  H   -0.028544  0.399486 -0.028544  0.003143  0.003143  0.459808
     7  H    0.003143 -0.028544  0.399486 -0.028544  0.003143 -0.001535
     8  H    0.003143  0.003143 -0.028544  0.399486 -0.028544 -0.000018
     9  H   -0.028544  0.003143  0.003143 -0.028544  0.399486 -0.000018
    10  H    0.399486 -0.028544  0.003143  0.003143 -0.028544 -0.001535
```

11	C	0.008245	-0.001791	-0.000649	-0.000649	-0.001791	-0.000036
12	C	-0.001791	0.008245	-0.001791	-0.000649	-0.000649	-0.000281
13	C	-0.000649	-0.001791	0.008245	-0.001791	-0.000649	-0.000036
14	C	-0.000649	-0.000649	-0.001791	0.008245	-0.001791	0.000000
15	C	-0.001791	-0.000649	-0.000649	-0.001791	0.008245	0.000000
16	H	-0.000281	-0.000036	0.000000	0.000000	-0.000036	0.000001
17	H	-0.000036	-0.000281	-0.000036	0.000000	0.000000	0.000007
18	H	0.000000	-0.000036	-0.000281	-0.000036	0.000000	0.000001
19	H	0.000000	0.000000	-0.000036	-0.000281	-0.000036	0.000000
20	H	-0.000036	0.000000	0.000000	-0.000036	-0.000281	0.000000
21	Ru	-0.014226	-0.014226	-0.014226	-0.014226	-0.014226	-0.005723

		7	8	9	10	11	12
1	C	0.003143	0.003143	-0.028544	0.399486	0.008245	-0.001791
2	C	-0.028544	0.003143	0.003143	-0.028544	-0.001791	0.008245
3	C	0.399486	-0.028544	0.003143	0.003143	-0.000649	-0.001791
4	C	-0.028544	0.399486	-0.028544	0.003143	-0.000649	-0.000649
5	C	0.003143	-0.028544	0.399486	-0.028544	-0.001791	-0.000649
6	H	-0.001535	-0.000018	-0.000018	-0.001535	-0.000036	-0.000281
7	H	0.459808	-0.001535	-0.000018	-0.000018	0.000000	-0.000036
8	H	-0.001535	0.459808	-0.001535	-0.000018	0.000000	0.000000
9	H	-0.000018	-0.001535	0.459808	-0.001535	-0.000036	0.000000
10	H	-0.000018	-0.000018	-0.001535	0.459808	-0.000281	-0.000036
11	C	0.000000	0.000000	-0.000036	-0.000281	5.473619	0.360190
12	C	-0.000036	0.000000	0.000000	-0.000036	0.360190	5.473619
13	C	-0.000281	-0.000036	0.000000	0.000000	-0.118533	0.360190
14	C	-0.000036	-0.000281	-0.000036	0.000000	-0.118533	-0.118533
15	C	0.000000	-0.000036	-0.000281	-0.000036	0.360190	-0.118533
16	H	0.000000	0.000000	0.000001	0.000007	0.399486	-0.028544
17	H	0.000001	0.000000	0.000000	0.000001	-0.028544	0.399486
18	H	0.000007	0.000001	0.000000	0.000000	0.003143	-0.028544
19	H	0.000001	0.000007	0.000001	0.000000	0.003143	0.003143
20	H	0.000000	0.000001	0.000007	0.000001	-0.028544	0.003143
21	Ru	-0.005723	-0.005723	-0.005723	-0.005723	-0.014226	-0.014226

		13	14	15	16	17	18
1	C	-0.000649	-0.000649	-0.001791	-0.000281	-0.000036	0.000000
2	C	-0.001791	-0.000649	-0.000649	-0.000036	-0.000281	-0.000036
3	C	0.008245	-0.001791	-0.000649	0.000000	-0.000036	-0.000281
4	C	-0.001791	0.008245	-0.001791	0.000000	0.000000	-0.000036
5	C	-0.000649	-0.001791	0.008245	-0.000036	0.000000	0.000000
6	H	-0.000036	0.000000	0.000000	0.000001	0.000007	0.000001
7	H	-0.000281	-0.000036	0.000000	0.000000	0.000001	0.000007
8	H	-0.000036	-0.000281	-0.000036	0.000000	0.000000	0.000001
9	H	0.000000	-0.000036	-0.000281	0.000001	0.000000	0.000000
10	H	0.000000	0.000000	-0.000036	0.000007	0.000001	0.000000
11	C	-0.118533	-0.118533	0.360190	0.399486	-0.028544	0.003143
12	C	0.360190	-0.118533	-0.118533	-0.028544	0.399486	-0.028544
13	C	5.473619	0.360190	-0.118533	0.003143	-0.028544	0.399486
14	C	0.360190	5.473619	0.360190	0.003143	0.003143	-0.028544
15	C	-0.118533	0.360190	5.473619	-0.028544	0.003143	0.003143
16	H	0.003143	0.003143	-0.028544	0.459808	-0.001535	-0.000018

17	H	-0.028544	0.003143	0.003143	-0.001535	0.459808	-0.001535
18	H	0.399486	-0.028544	0.003143	-0.000018	-0.001535	0.459808
19	H	-0.028544	0.399486	-0.028544	-0.000018	-0.000018	-0.001535
20	H	0.003143	-0.028544	0.399486	-0.001535	-0.000018	-0.000018
21	Ru	-0.014226	-0.014226	-0.014226	-0.005723	-0.005723	-0.005723

		19	20	21
1	C	0.000000	-0.000036	-0.014226
2	C	0.000000	0.000000	-0.014226
3	C	-0.000036	0.000000	-0.014226
4	C	-0.000281	-0.000036	-0.014226
5	C	-0.000036	-0.000281	-0.014226
6	H	0.000000	0.000000	-0.005723
7	H	0.000001	0.000000	-0.005723
8	H	0.000007	0.000001	-0.005723
9	H	0.000001	0.000007	-0.005723
10	H	0.000000	0.000001	-0.005723
11	C	0.003143	-0.028544	-0.014226
12	C	0.003143	0.003143	-0.014226
13	C	-0.028544	0.003143	-0.014226
14	C	0.399486	-0.028544	-0.014226
15	C	-0.028544	0.399486	-0.014226
16	H	-0.000018	-0.001535	-0.005723
17	H	-0.000018	-0.000018	-0.005723
18	H	-0.001535	-0.000018	-0.005723
19	H	0.459808	-0.001535	-0.005723
20	H	-0.001535	0.459808	-0.005723
21	Ru	-0.005723	-0.005723	43.262230

Mulliken charges:

		1
1	C	-0.294403
2	C	-0.294403
3	C	-0.294403
4	C	-0.294403
5	C	-0.294403
6	H	0.200678
7	H	0.200678
8	H	0.200678
9	H	0.200678
10	H	0.200678
11	C	-0.294403
12	C	-0.294403
13	C	-0.294403
14	C	-0.294403
15	C	-0.294403
16	H	0.200678
17	H	0.200678
18	H	0.200678
19	H	0.200678
20	H	0.200678
21	Ru	0.937253

Sum of Mulliken charges = -0.00000
Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	-0.093725
2	C	-0.093725
3	C	-0.093725
4	C	-0.093725
5	C	-0.093725
11	C	-0.093725
12	C	-0.093725
13	C	-0.093725
14	C	-0.093725
15	C	-0.093725
21	Ru	0.937253

APT charges:

		1
1	C	0.003282
2	C	0.003269
3	C	0.003277
4	C	0.003277
5	C	0.003269
6	H	0.047981
7	H	0.047981
8	H	0.047981
9	H	0.047981
10	H	0.047979
11	C	0.003282
12	C	0.003269
13	C	0.003277
14	C	0.003277
15	C	0.003269
16	H	0.047979
17	H	0.047981
18	H	0.047981
19	H	0.047981
20	H	0.047981
21	Ru	-0.512472

Sum of APT charges =   0.00008
APT charges with hydrogens summed into heavy atoms:

		1
1	C	0.051261
2	C	0.051250
3	C	0.051258
4	C	0.051258
5	C	0.051250
11	C	0.051261
12	C	0.051250
13	C	0.051258
14	C	0.051258
15	C	0.051250

```
    21  Ru  -0.512472
 Electronic spatial extent (au):  <R**2>=           1580.3475
 Charge=              -0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=              0.0000    Y=              0.0000    Z=              0.0000
Tot=              0.0000
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=            -75.0030   YY=            -75.0030   ZZ=            -87.9294
   XY=              0.0000   XZ=             -0.0000   YZ=              0.0000
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=              4.3088   YY=              4.3088   ZZ=             -8.6176
   XY=              0.0000   XZ=             -0.0000   YZ=              0.0000
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=              0.0000  YYY=              0.0000  ZZZ=             -0.0000
XYY=             -0.0000
  XXY=             -0.0000  XXZ=              0.0000  XZZ=              0.0000
YZZ=              0.0000
  YYZ=              0.0000  XYZ=              0.0000
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=           -384.4337 YYYY=           -384.4337 ZZZZ=          -1523.7071
XXXY=              0.0000
 XXXZ=             -0.0000 YYYX=              0.0000 YYYZ=             -0.0000
ZZZX=             -0.0000
 ZZZY=             -0.0000 XXYY=           -128.1446 XXZZ=           -275.0281
YYZZ=           -275.0281
 XXYZ=              0.0000 YYXZ=              0.0000 ZZXY=              0.0000
 N-N= 1.146176580660D+03 E-N=-1.369676243591D+04  KE= 4.784544651090D+03
 Symmetry A1   KE= 3.197824744599D+03
 Symmetry A2   KE= 1.702475655609D+02
 Symmetry B1   KE= 6.923190071018D+02
 Symmetry B2   KE= 7.241533338283D+02
  Exact polarizability: 101.201  -0.000 101.201  -0.000  -0.000 142.749
 Approx polarizability: 175.218   0.000 175.218  -0.000  -0.000 264.452
 Calling FoFJK, ICntrl=    100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
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 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
 Defaulting to unpruned grid for atomic number  44.
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Defaulting to unpruned grid for atomic number  44.
Full mass-weighted force constant matrix:
Low frequencies ---   -0.0037    0.0122    0.0163    6.5453    6.5463    6.6338
Low frequencies ---   39.1303  145.2559  145.2573
Diagonal vibrational polarizability:
       5.5115870       5.5118512       5.7441360
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:
                     1                      2                      3
                    A1"                    E1'                    E1'
Frequencies --     39.1303               145.2559               145.2573
Red. masses --      3.4339                 4.8030                 4.8030
Frc consts  --      0.0031                 0.0597                 0.0597
IR Inten    --      0.0000                 1.4361                 1.4358
 Atom  AN      X      Y      Z        X      Y      Z        X      Y      Z
    1   6     0.15  -0.00   0.00     0.00  -0.08   0.19    -0.08  -0.00   0.00
    2   6     0.05  -0.14   0.00    -0.00  -0.08   0.06    -0.08  -0.00   0.18
    3   6    -0.12  -0.09   0.00     0.00  -0.08  -0.15    -0.08   0.00   0.11
    4   6    -0.12   0.09  -0.00    -0.00  -0.08  -0.15    -0.08  -0.00  -0.11
    5   6     0.05   0.14  -0.00     0.00  -0.08   0.06    -0.08   0.00  -0.18
    6   1     0.09  -0.27   0.00    -0.00  -0.09   0.11    -0.09  -0.00   0.35
    7   1    -0.23  -0.16  -0.00     0.00  -0.09  -0.30    -0.09   0.00   0.21
    8   1    -0.23   0.16  -0.00    -0.00  -0.09  -0.30    -0.09  -0.00  -0.21
    9   1     0.09   0.27  -0.00     0.00  -0.09   0.11    -0.09   0.00  -0.35
   10   1     0.28  -0.00   0.00     0.00  -0.09   0.37    -0.09  -0.00   0.00
   11   6    -0.15  -0.00  -0.00     0.00  -0.08  -0.19    -0.08  -0.00  -0.00
   12   6    -0.05   0.14   0.00    -0.00  -0.08  -0.06    -0.08  -0.00  -0.18
   13   6     0.12   0.09   0.00     0.00  -0.08   0.15    -0.08   0.00  -0.11
   14   6     0.12  -0.09  -0.00    -0.00  -0.08   0.15    -0.08  -0.00   0.11
   15   6    -0.05  -0.14  -0.00     0.00  -0.08  -0.06    -0.08   0.00   0.18
   16   1    -0.28  -0.00  -0.00     0.00  -0.09  -0.37    -0.09  -0.00  -0.00
   17   1    -0.09   0.27   0.00    -0.00  -0.09  -0.11    -0.09  -0.00  -0.35
   18   1     0.23   0.16   0.00     0.00  -0.09   0.30    -0.09   0.00  -0.21
   19   1     0.23  -0.16   0.00    -0.00  -0.09   0.30    -0.09  -0.00   0.21
   20   1    -0.09  -0.27  -0.00     0.00  -0.09  -0.11    -0.09   0.00   0.35
   21  44    -0.00   0.00   0.00    -0.00   0.11  -0.00     0.11   0.00   0.00
                     4                      5                      6
                    A1'                    E1"                    E1"
Frequencies --    307.8369               355.4400               355.4402
Red. masses --      5.5671                 4.6377                 4.6377
Frc consts  --      0.3108                 0.3452                 0.3452
IR Inten    --      0.0000                 0.0000                 0.0000
 Atom  AN      X      Y      Z        X      Y      Z        X      Y      Z
    1   6    -0.00  -0.01   0.20    -0.10   0.00   0.00     0.00   0.07   0.23
    2   6    -0.01  -0.00   0.20    -0.07   0.01  -0.22    -0.01   0.09   0.07
    3   6    -0.01   0.01   0.20    -0.09  -0.01  -0.13     0.01   0.08  -0.18
    4   6     0.01   0.01   0.20    -0.09   0.01   0.13    -0.01   0.08  -0.18
    5   6     0.01  -0.00   0.20    -0.07  -0.01   0.22     0.01   0.09   0.07
```

6	1	-0.01	-0.00	0.24	-0.07	0.01	-0.32	-0.01	0.11	0.11
7	1	-0.01	0.01	0.24	-0.10	-0.02	-0.20	0.02	0.08	-0.28
8	1	0.01	0.01	0.24	-0.10	0.02	0.20	-0.02	0.08	-0.28
9	1	0.01	-0.00	0.24	-0.07	-0.01	0.32	0.01	0.11	0.11
10	1	-0.00	-0.01	0.24	-0.11	0.00	0.00	0.00	0.07	0.34
11	6	0.00	-0.01	-0.20	0.10	-0.00	0.00	-0.00	-0.07	0.23
12	6	-0.01	-0.00	-0.20	0.07	-0.01	-0.22	0.01	-0.09	0.07
13	6	-0.01	0.01	-0.20	0.09	0.01	-0.13	-0.01	-0.08	-0.18
14	6	0.01	0.01	-0.20	0.09	-0.01	0.13	0.01	-0.08	-0.18
15	6	0.01	-0.00	-0.20	0.07	0.01	0.22	-0.01	-0.09	0.07
16	1	0.00	-0.01	-0.24	0.11	-0.00	0.00	0.00	-0.07	0.34
17	1	-0.01	-0.00	-0.24	0.07	-0.01	-0.32	0.01	-0.11	0.11
18	1	-0.01	0.01	-0.24	0.10	0.02	-0.20	-0.02	-0.08	-0.28
19	1	0.01	0.01	-0.24	0.10	-0.02	0.20	0.02	-0.08	-0.28
20	1	0.01	-0.00	-0.24	0.07	0.01	0.32	-0.01	-0.11	0.11
21	44	-0.00	0.00	-0.00	0.00	0.00	-0.00	-0.00	-0.00	0.00

	7	8	9
	A2"	E1'	E1'
Frequencies --	375.9774	421.6191	421.6195
Red. masses --	10.1040	9.0319	9.0318
Frc consts --	0.8415	0.9459	0.9460
IR Inten --	0.0936	20.3848	20.3840

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.03	-0.18	-0.15	0.00	0.00	-0.00	-0.11	-0.25
2	6	0.02	0.01	-0.18	-0.11	0.01	-0.23	0.01	-0.15	-0.08
3	6	0.02	-0.02	-0.18	-0.14	-0.02	-0.15	-0.02	-0.12	0.20
4	6	-0.02	-0.02	-0.18	-0.14	0.02	0.15	0.02	-0.12	0.20
5	6	-0.02	0.01	-0.18	-0.11	-0.01	0.23	-0.01	-0.15	-0.08
6	1	0.03	0.01	-0.25	-0.12	0.02	-0.21	0.02	-0.19	-0.07
7	1	0.02	-0.02	-0.25	-0.16	-0.04	-0.13	-0.04	-0.14	0.18
8	1	-0.02	-0.02	-0.25	-0.16	0.04	0.13	0.04	-0.14	0.18
9	1	-0.03	0.01	-0.25	-0.12	-0.02	0.21	-0.02	-0.19	-0.07
10	1	0.00	0.03	-0.25	-0.19	0.00	0.00	-0.00	-0.11	-0.22
11	6	0.00	-0.03	-0.18	-0.15	0.00	-0.00	-0.00	-0.11	0.25
12	6	-0.02	-0.01	-0.18	-0.11	0.01	0.23	0.01	-0.15	0.08
13	6	-0.02	0.02	-0.18	-0.14	-0.02	0.15	-0.02	-0.12	-0.20
14	6	0.02	0.02	-0.18	-0.14	0.02	-0.15	0.02	-0.12	-0.20
15	6	0.02	-0.01	-0.18	-0.11	-0.01	-0.23	-0.01	-0.15	0.08
16	1	0.00	-0.03	-0.25	-0.19	0.00	-0.00	-0.00	-0.11	0.22
17	1	-0.03	-0.01	-0.25	-0.12	0.02	0.21	0.02	-0.19	0.07
18	1	-0.02	0.02	-0.25	-0.16	-0.04	0.13	-0.04	-0.14	-0.18
19	1	0.02	0.02	-0.25	-0.16	0.04	-0.13	0.04	-0.14	-0.18
20	1	0.03	-0.01	-0.25	-0.12	-0.02	-0.21	-0.02	-0.19	0.07
21	44	-0.00	-0.00	0.23	0.17	-0.00	0.00	0.00	0.17	0.00

	10	11	12
	E2"	E2"	E2'
Frequencies --	567.2379	567.2380	581.2365
Red. masses --	4.8130	4.8130	4.8069
Frc consts --	0.9124	0.9124	0.9568
IR Inten --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.26	-0.03	0.00	0.00	0.00	-0.01	0.26
2	6	-0.01	0.01	-0.21	0.00	-0.02	-0.15	0.01	0.01	-0.21
3	6	-0.02	-0.02	0.08	0.01	0.00	0.25	-0.01	-0.00	0.08
4	6	0.02	-0.02	0.08	0.01	-0.00	-0.25	0.01	-0.00	0.08
5	6	0.01	0.01	-0.21	0.00	0.02	0.15	-0.01	0.01	-0.21
6	1	-0.01	0.01	-0.29	0.00	-0.02	-0.21	0.01	0.01	-0.29
7	1	-0.02	-0.01	0.11	0.01	0.00	0.34	-0.02	-0.01	0.11
8	1	0.02	-0.01	0.11	0.01	-0.00	-0.34	0.02	-0.01	0.11
9	1	0.01	0.01	-0.29	0.00	0.02	0.21	-0.01	0.01	-0.29
10	1	-0.00	0.00	0.36	-0.02	0.00	0.00	0.00	-0.01	0.36
11	6	0.00	-0.00	0.26	0.03	0.00	-0.00	-0.00	-0.01	-0.26
12	6	0.01	-0.01	-0.21	-0.00	0.02	-0.15	0.01	0.01	0.21
13	6	0.02	0.02	0.08	-0.01	-0.00	0.25	-0.01	-0.00	-0.08
14	6	-0.02	0.02	0.08	-0.01	0.00	-0.25	0.01	-0.00	-0.08
15	6	-0.01	-0.01	-0.21	-0.00	-0.02	0.15	-0.01	0.01	0.21
16	1	0.00	-0.00	0.36	0.02	0.00	-0.00	-0.00	-0.01	-0.36
17	1	0.01	-0.01	-0.29	-0.00	0.02	-0.21	0.01	0.01	0.29
18	1	0.02	0.01	0.11	-0.01	-0.00	0.34	-0.02	-0.01	-0.11
19	1	-0.02	0.01	0.11	-0.01	0.00	-0.34	0.02	-0.01	-0.11
20	1	-0.01	-0.01	-0.29	-0.00	-0.02	0.21	-0.01	0.01	0.29
21	44	0.00	0.00	0.00	-0.00	-0.00	0.00	0.00	-0.00	0.00

	13	14	15
	E2'	A2"	E1"
Frequencies --	581.2367	804.3118	805.6326
Red. masses --	4.8069	1.1185	1.1984
Frc consts --	0.9568	0.4263	0.4583
IR Inten --	0.0000	129.2808	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	0.00	-0.00	0.00	-0.00	-0.03	0.00	0.01	-0.06
2	6	0.01	-0.00	-0.15	-0.00	-0.00	-0.03	0.00	0.00	-0.02
3	6	-0.00	0.01	0.25	-0.00	0.00	-0.03	-0.00	0.01	0.05
4	6	-0.00	-0.01	-0.25	0.00	0.00	-0.03	0.00	0.01	0.05
5	6	0.01	0.00	0.15	0.00	-0.00	-0.03	-0.00	0.00	-0.02
6	1	0.01	-0.01	-0.21	-0.02	-0.01	0.31	-0.00	-0.01	0.14
7	1	-0.00	0.01	0.34	-0.01	0.01	0.31	0.00	-0.01	-0.36
8	1	-0.00	-0.01	-0.34	0.01	0.01	0.31	-0.00	-0.01	-0.36
9	1	0.01	0.01	0.21	0.02	-0.01	0.31	0.00	-0.01	0.14
10	1	-0.02	0.00	-0.00	-0.00	-0.02	0.31	-0.00	-0.01	0.44
11	6	-0.01	-0.00	0.00	0.00	0.00	-0.03	0.00	-0.01	-0.06
12	6	0.01	-0.00	0.15	0.00	0.00	-0.03	-0.00	-0.00	-0.02
13	6	-0.00	0.01	-0.25	0.00	-0.00	-0.03	0.00	-0.01	0.05
14	6	-0.00	-0.01	0.25	-0.00	-0.00	-0.03	-0.00	-0.01	0.05
15	6	0.01	0.00	-0.15	-0.00	0.00	-0.03	0.00	-0.00	-0.02
16	1	-0.02	-0.00	-0.00	-0.00	0.02	0.31	-0.00	0.01	0.44
17	1	0.01	-0.01	0.21	0.02	0.01	0.31	0.00	0.01	0.14
18	1	-0.00	0.01	-0.34	0.01	-0.01	0.31	-0.00	0.01	-0.36
19	1	-0.00	-0.01	0.34	-0.01	-0.01	0.31	0.00	0.01	-0.36
20	1	0.01	0.01	-0.21	-0.02	0.01	0.31	-0.00	0.01	0.14
21	44	0.00	0.00	-0.00	-0.00	-0.00	0.01	0.00	-0.00	-0.00

		16			17			18		
		E1"			A1'			E1'		
Frequencies --		805.6329			815.8780			838.1981		
Red. masses --		1.1984			1.1201			1.1921		
Frc consts --		0.4583			0.4393			0.4935		
IR Inten --		0.0000			0.0000			0.0021		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.00	0.00	0.00	0.00	-0.00	-0.03	0.00	0.01	-0.06
2	6	0.01	0.00	-0.06	-0.00	-0.00	-0.03	-0.00	0.01	-0.02
3	6	0.00	-0.00	-0.03	-0.00	0.00	-0.03	0.00	0.01	0.04
4	6	0.00	0.00	0.03	0.00	0.00	-0.03	-0.00	0.01	0.04
5	6	0.01	-0.00	0.06	0.00	-0.00	-0.03	0.00	0.01	-0.02
6	1	-0.01	-0.00	0.42	-0.02	-0.01	0.31	-0.01	0.02	0.14
7	1	-0.01	0.00	0.26	-0.01	0.01	0.31	0.02	0.00	-0.36
8	1	-0.01	-0.00	-0.26	0.01	0.01	0.31	-0.02	0.00	-0.36
9	1	-0.01	0.00	-0.42	0.02	-0.01	0.31	0.01	0.02	0.14
10	1	-0.01	0.00	-0.00	-0.00	-0.02	0.31	-0.00	-0.01	0.44
11	6	0.00	0.00	-0.00	-0.00	-0.00	0.03	-0.00	0.01	0.06
12	6	-0.01	-0.00	-0.06	-0.00	-0.00	0.03	-0.00	0.01	0.02
13	6	-0.00	0.00	-0.03	-0.00	0.00	0.03	0.00	0.01	-0.04
14	6	-0.00	-0.00	0.03	0.00	0.00	0.03	-0.00	0.01	-0.04
15	6	-0.01	0.00	0.06	0.00	-0.00	0.03	0.00	0.01	0.02
16	1	0.01	0.00	0.00	0.00	-0.02	-0.31	0.00	-0.01	-0.44
17	1	0.01	0.00	0.42	-0.02	-0.01	-0.31	-0.01	0.02	-0.14
18	1	0.01	-0.00	0.26	-0.01	0.01	-0.31	0.02	0.00	0.36
19	1	0.01	0.00	-0.26	0.01	0.01	-0.31	-0.02	0.00	0.36
20	1	0.01	-0.00	-0.42	0.02	-0.01	-0.31	0.01	0.02	-0.14
21	44	-0.00	0.00	-0.00	-0.00	-0.00	-0.00	-0.00	-0.01	0.00

		19			20			21		
		E1'			E2"			E2"		
Frequencies --		838.1984			843.6836			843.6836		
Red. masses --		1.1921			3.9892			3.9893		
Frc consts --		0.4935			1.6730			1.6731		
IR Inten --		0.0021			0.0000			0.0000		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.01	-0.00	0.00	-0.00	0.21	-0.04	-0.09	-0.00	-0.00
2	6	-0.01	0.00	0.05	-0.18	-0.00	0.04	-0.09	-0.11	0.03
3	6	-0.01	-0.00	0.03	-0.03	-0.10	-0.01	0.14	-0.14	-0.04
4	6	-0.01	0.00	-0.03	0.03	-0.10	-0.01	0.14	0.14	0.04
5	6	-0.01	-0.00	-0.05	0.18	-0.00	0.04	-0.09	0.11	-0.03
6	1	0.01	0.01	-0.42	-0.12	-0.13	-0.24	-0.15	0.08	-0.17
7	1	-0.01	-0.02	-0.26	0.15	0.03	0.09	0.07	-0.18	0.28
8	1	-0.01	0.02	0.26	-0.15	0.03	0.09	0.07	0.18	-0.28
9	1	0.01	-0.01	0.42	0.12	-0.13	-0.24	-0.15	-0.08	0.17
10	1	-0.03	-0.00	-0.00	-0.00	0.20	0.29	0.15	-0.00	0.00
11	6	-0.01	0.00	0.00	-0.00	-0.21	-0.04	0.09	0.00	0.00
12	6	-0.01	0.00	-0.05	0.18	0.00	0.04	0.09	0.11	0.03
13	6	-0.01	-0.00	-0.03	0.03	0.10	-0.01	-0.14	0.14	-0.04
14	6	-0.01	0.00	0.03	-0.03	0.10	-0.01	-0.14	-0.14	0.04
15	6	-0.01	-0.00	0.05	-0.18	0.00	0.04	0.09	-0.11	-0.03

16	1	-0.03	0.00	-0.00	-0.00	-0.20	0.29	-0.15	-0.00	-0.00
17	1	0.01	0.01	0.42	0.12	0.13	-0.24	0.15	-0.08	-0.17
18	1	-0.01	-0.02	0.26	-0.15	-0.03	0.09	-0.07	0.18	0.28
19	1	-0.01	0.02	-0.26	0.15	-0.03	0.09	-0.07	-0.18	-0.28
20	1	0.01	-0.01	-0.42	-0.12	0.13	-0.24	0.15	0.08	0.17
21	44	0.01	-0.00	0.00	0.00	-0.00	0.00	0.00	-0.00	-0.00

	22	23	24
	E2'	E2'	E2"
Frequencies --	866.9928	866.9930	872.8500
Red. masses --	2.8733	2.8733	1.2801
Frc consts --	1.2725	1.2725	0.5746
IR Inten --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.07	-0.00	-0.00	0.00	0.17	-0.03	-0.03	0.00	-0.00
2	6	0.08	0.08	-0.02	-0.14	-0.01	0.03	-0.01	-0.03	-0.03
3	6	-0.11	0.12	0.03	-0.02	-0.08	-0.01	0.03	-0.02	0.04
4	6	-0.11	-0.12	-0.03	0.02	-0.08	-0.01	0.03	0.02	-0.04
5	6	0.08	-0.08	0.02	0.14	-0.01	0.03	-0.01	0.03	0.03
6	1	0.12	-0.08	0.21	-0.09	-0.12	-0.28	-0.04	0.01	0.26
7	1	-0.05	0.14	-0.33	0.13	0.04	0.11	0.03	-0.05	-0.42
8	1	-0.05	-0.14	0.33	-0.13	0.04	0.11	0.03	0.05	0.42
9	1	0.12	0.08	-0.21	0.09	-0.12	-0.28	-0.04	-0.01	-0.26
10	1	-0.14	-0.00	0.00	-0.00	0.15	0.35	0.02	0.00	0.00
11	6	0.07	0.00	-0.00	-0.00	0.17	0.03	0.03	0.00	0.00
12	6	0.08	0.08	0.02	-0.14	-0.01	-0.03	0.01	0.03	-0.03
13	6	-0.11	0.12	-0.03	-0.02	-0.08	0.01	-0.03	0.02	0.04
14	6	-0.11	-0.12	0.03	0.02	-0.08	0.01	-0.03	-0.02	-0.04
15	6	0.08	-0.08	-0.02	0.14	-0.01	-0.03	0.01	-0.03	0.03
16	1	-0.14	0.00	0.00	0.00	0.15	-0.35	-0.02	0.00	-0.00
17	1	0.12	-0.08	-0.21	-0.09	-0.12	0.28	0.04	-0.01	0.26
18	1	-0.05	0.14	0.33	0.13	0.04	-0.11	-0.03	0.05	-0.42
19	1	-0.05	-0.14	-0.33	-0.13	0.04	-0.11	-0.03	-0.05	0.42
20	1	0.12	0.08	0.21	0.09	-0.12	0.28	0.04	0.01	-0.26
21	44	0.00	0.00	-0.00	0.00	-0.00	0.00	-0.00	-0.00	-0.00

	25	26	27
	E2"	E2'	E2'
Frequencies --	872.8510	886.1907	886.1918
Red. masses --	1.2801	1.4286	1.4286
Frc consts --	0.5746	0.6610	0.6610
IR Inten --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.00	-0.04	-0.05	0.04	-0.00	0.00	0.00	-0.06	-0.05
2	6	0.04	-0.01	0.04	0.03	0.04	0.03	0.05	-0.00	0.04
3	6	0.02	0.03	-0.01	-0.04	0.04	-0.05	0.02	0.04	-0.02
4	6	-0.02	0.03	-0.01	-0.04	-0.04	0.05	-0.02	0.04	-0.02
5	6	-0.04	-0.01	0.04	0.03	-0.04	-0.03	-0.05	-0.00	0.04
6	1	0.04	0.03	-0.35	0.06	-0.03	-0.25	0.05	0.05	-0.35
7	1	-0.03	0.00	0.13	-0.03	0.07	0.41	-0.06	-0.01	0.13
8	1	0.03	0.00	0.13	-0.03	-0.07	-0.41	0.06	-0.01	0.13
9	1	-0.04	0.03	-0.35	0.06	0.03	0.25	-0.05	0.05	-0.35

10	1	0.00	-0.06	0.44	-0.05	-0.00	-0.00	0.00	-0.08	0.43
11	6	-0.00	0.04	-0.05	0.04	0.00	0.00	-0.00	-0.06	0.05
12	6	-0.04	0.01	0.04	0.03	0.04	-0.03	0.05	-0.00	-0.04
13	6	-0.02	-0.03	-0.01	-0.04	0.04	0.05	0.02	0.04	0.02
14	6	0.02	-0.03	-0.01	-0.04	-0.04	-0.05	-0.02	0.04	0.02
15	6	0.04	0.01	0.04	0.03	-0.04	0.03	-0.05	-0.00	-0.04
16	1	0.00	0.06	0.44	-0.05	0.00	-0.00	-0.00	-0.08	-0.43
17	1	-0.04	-0.03	-0.35	0.06	-0.03	0.25	0.05	0.05	0.35
18	1	0.03	-0.00	0.13	-0.03	0.07	-0.41	-0.06	-0.01	-0.13
19	1	-0.03	-0.00	0.13	-0.03	-0.07	0.41	0.06	-0.01	-0.13
20	1	0.04	-0.03	-0.35	0.06	0.03	-0.25	-0.05	0.05	0.35
21	44	-0.00	-0.00	-0.00	-0.00	0.00	-0.00	0.00	0.00	0.00

	28	29	30
	E1"	E1"	E1'
Frequencies --	1010.1364	1010.1368	1018.7266
Red. masses --	1.6434	1.6434	1.6428
Frc consts --	0.9880	0.9880	1.0045
IR Inten --	0.0000	0.0000	18.0988

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.06	-0.00	-0.00	0.00	-0.09	-0.01	0.05	0.00	0.00
2	6	-0.08	-0.04	-0.01	-0.04	0.04	-0.00	-0.08	-0.04	-0.01
3	6	0.01	0.07	-0.01	0.07	-0.04	0.01	0.00	0.07	-0.00
4	6	0.01	-0.07	0.01	-0.07	-0.04	0.01	0.00	-0.07	0.00
5	6	-0.08	0.04	0.01	0.04	0.04	-0.00	-0.08	0.04	0.01
6	1	-0.05	-0.15	0.01	-0.15	0.37	0.00	-0.05	-0.15	-0.03
7	1	0.24	0.25	0.01	0.25	0.08	-0.01	0.24	0.25	-0.02
8	1	0.24	-0.25	-0.01	-0.25	0.08	-0.01	0.24	-0.25	0.02
9	1	-0.05	0.15	-0.01	0.15	0.37	0.00	-0.05	0.15	0.03
10	1	0.42	-0.00	-0.00	0.00	-0.10	0.01	0.42	0.00	0.00
11	6	-0.06	-0.00	0.00	0.00	0.09	-0.01	0.05	-0.00	0.00
12	6	0.08	0.04	-0.01	0.04	-0.04	-0.00	-0.08	-0.04	0.01
13	6	-0.01	-0.07	-0.01	-0.07	0.04	0.01	0.00	0.07	0.00
14	6	-0.01	0.07	0.01	0.07	0.04	0.01	0.00	-0.07	-0.00
15	6	0.08	-0.04	0.01	-0.04	-0.04	-0.00	-0.08	0.04	-0.01
16	1	-0.42	-0.00	0.00	0.00	0.10	0.01	0.42	-0.00	-0.00
17	1	0.05	0.15	0.01	0.15	-0.37	0.00	-0.05	-0.15	0.03
18	1	-0.24	-0.25	0.01	-0.25	-0.08	-0.01	0.24	0.25	0.02
19	1	-0.24	0.25	-0.01	0.25	-0.08	-0.01	0.24	-0.25	-0.02
20	1	0.05	-0.15	-0.01	-0.15	-0.37	0.00	-0.05	0.15	-0.03
21	44	-0.00	0.00	-0.00	0.00	-0.00	-0.00	0.01	-0.00	-0.00

	31	32	33
	E1'	E2"	E2"
Frequencies --	1018.7270	1084.2353	1084.2353
Red. masses --	1.6428	1.2504	1.2504
Frc consts --	1.0045	0.8661	0.8661
IR Inten --	18.0972	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.00	-0.09	-0.01	0.07	-0.00	-0.00	0.00	0.01	0.01
2	6	-0.04	0.04	-0.00	-0.02	0.05	-0.01	0.01	-0.04	-0.01
3	6	0.07	-0.04	0.01	-0.01	-0.02	0.01	0.05	0.03	0.00

4	6	-0.07	-0.04	0.01	-0.01	0.02	-0.01	-0.05	0.03	0.00
5	6	0.04	0.04	-0.00	-0.02	-0.05	0.01	-0.01	-0.04	-0.01
6	1	-0.15	0.37	-0.01	-0.11	0.34	0.01	0.07	-0.25	0.01
7	1	0.25	0.08	0.02	-0.11	-0.09	-0.02	0.34	0.25	-0.01
8	1	-0.25	0.08	0.02	-0.11	0.09	0.02	-0.34	0.25	-0.01
9	1	0.15	0.37	-0.01	-0.11	-0.34	-0.01	-0.07	-0.25	0.01
10	1	-0.00	-0.10	-0.03	0.44	-0.00	-0.00	0.00	0.01	-0.02
11	6	0.00	-0.09	0.01	-0.07	-0.00	0.00	-0.00	-0.01	0.01
12	6	-0.04	0.04	0.00	0.02	-0.05	-0.01	-0.01	0.04	-0.01
13	6	0.07	-0.04	-0.01	0.01	0.02	0.01	-0.05	-0.03	0.00
14	6	-0.07	-0.04	-0.01	0.01	-0.02	-0.01	0.05	-0.03	0.00
15	6	0.04	0.04	0.00	0.02	0.05	0.01	0.01	0.04	-0.01
16	1	0.00	-0.10	0.03	-0.44	-0.00	0.00	0.00	-0.01	-0.02
17	1	-0.15	0.37	0.01	0.11	-0.34	0.01	-0.07	0.25	0.01
18	1	0.25	0.08	-0.02	0.11	0.09	-0.02	-0.34	-0.25	-0.01
19	1	-0.25	0.08	-0.02	0.11	-0.09	0.02	0.34	-0.25	-0.01
20	1	0.15	0.37	0.01	0.11	0.34	-0.01	0.07	0.25	0.01
21	44	0.00	0.01	-0.00	-0.00	0.00	-0.00	-0.00	0.00	0.00

	34	35	36
	E2'	E2'	A1'
Frequencies --	1096.1667	1096.1667	1109.7897
Red. masses --	1.2257	1.2257	5.7093
Frc consts --	0.8677	0.8677	4.1430
IR Inten --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.06	-0.00	-0.00	-0.00	0.00	-0.01	0.00	0.21	0.01
2	6	-0.01	0.05	-0.00	-0.01	0.03	0.00	0.20	0.06	0.01
3	6	-0.02	-0.01	0.01	-0.05	-0.04	-0.00	0.12	-0.17	0.01
4	6	-0.02	0.01	-0.01	0.05	-0.04	-0.00	-0.12	-0.17	0.01
5	6	-0.01	-0.05	0.00	0.01	0.03	0.00	-0.20	0.06	0.01
6	1	-0.11	0.34	0.00	-0.08	0.25	-0.01	0.22	0.07	0.06
7	1	-0.11	-0.08	-0.01	-0.34	-0.25	0.00	0.14	-0.19	0.06
8	1	-0.11	0.08	0.01	0.34	-0.25	0.00	-0.14	-0.19	0.06
9	1	-0.11	-0.34	-0.00	0.08	0.25	-0.01	-0.22	0.07	0.06
10	1	0.44	-0.00	-0.00	-0.00	0.00	0.01	0.00	0.23	0.06
11	6	0.06	0.00	-0.00	-0.00	0.00	0.01	-0.00	0.21	-0.01
12	6	-0.01	0.05	0.00	-0.01	0.03	-0.00	0.20	0.06	-0.01
13	6	-0.02	-0.01	-0.01	-0.05	-0.04	0.00	0.12	-0.17	-0.01
14	6	-0.02	0.01	0.01	0.05	-0.04	0.00	-0.12	-0.17	-0.01
15	6	-0.01	-0.05	-0.00	0.01	0.03	-0.00	-0.20	0.06	-0.01
16	1	0.44	0.00	-0.00	-0.00	0.00	-0.01	-0.00	0.23	-0.06
17	1	-0.11	0.34	-0.00	-0.08	0.25	0.01	0.22	0.07	-0.06
18	1	-0.11	-0.08	0.01	-0.34	-0.25	-0.00	0.14	-0.19	-0.06
19	1	-0.11	0.08	-0.01	0.34	-0.25	-0.00	-0.14	-0.19	-0.06
20	1	-0.11	-0.34	0.00	0.08	0.25	0.01	-0.22	0.07	-0.06
21	44	0.00	-0.00	0.00	0.00	-0.00	-0.00	-0.00	0.00	0.00

	37	38	39
	A2"	A1"	A2'
Frequencies --	1114.6062	1312.1481	1312.2344
Red. masses --	5.7394	1.2749	1.2751

Frc consts --		4.2010			1.2933			1.2936		
IR Inten --		15.7020			0.0000			0.0000		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.21	0.01	-0.05	0.00	0.00	-0.05	0.00	-0.00
2	6	0.20	0.06	0.01	-0.02	0.05	-0.00	-0.02	0.05	-0.00
3	6	0.12	-0.17	0.01	0.04	0.03	-0.00	0.04	0.03	-0.00
4	6	-0.12	-0.17	0.01	0.04	-0.03	-0.00	0.04	-0.03	-0.00
5	6	-0.20	0.06	0.01	-0.02	-0.05	0.00	-0.02	-0.05	0.00
6	1	0.22	0.07	0.05	0.10	-0.30	0.00	0.10	-0.30	0.00
7	1	0.14	-0.19	0.05	-0.25	-0.18	0.00	-0.25	-0.18	0.00
8	1	-0.14	-0.19	0.05	-0.25	0.18	0.00	-0.25	0.18	0.00
9	1	-0.22	0.07	0.05	0.10	0.30	-0.00	0.10	0.30	-0.00
10	1	0.00	0.23	0.05	0.31	0.00	0.00	0.31	0.00	0.00
11	6	0.00	-0.21	0.01	0.05	0.00	-0.00	-0.05	-0.00	-0.00
12	6	-0.20	-0.06	0.01	0.02	-0.05	-0.00	-0.02	0.05	0.00
13	6	-0.12	0.17	0.01	-0.04	-0.03	0.00	0.04	0.03	-0.00
14	6	0.12	0.17	0.01	-0.04	0.03	0.00	0.04	-0.03	-0.00
15	6	0.20	-0.06	0.01	0.02	0.05	0.00	-0.02	-0.05	-0.00
16	1	0.00	-0.23	0.05	-0.31	0.00	-0.00	0.31	-0.00	0.00
17	1	-0.22	-0.07	0.05	-0.10	0.30	0.00	0.10	-0.30	-0.00
18	1	-0.14	0.19	0.05	0.25	0.18	-0.00	-0.25	-0.18	0.00
19	1	0.14	0.19	0.05	0.25	-0.18	-0.00	-0.25	0.18	0.00
20	1	0.22	-0.07	0.05	-0.10	-0.30	-0.00	0.10	0.30	0.00
21	44	-0.00	0.00	-0.02	-0.00	-0.00	0.00	0.00	0.00	-0.00
		40			41			42		
		E2"			E2"			E2'		
Frequencies --		1343.5418			1343.5418			1365.9905		
Red. masses --		3.7160			3.7160			4.2184		
Frc consts --		3.9521			3.9521			4.6375		
IR Inten --		0.0000			0.0000			0.0000		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.11	0.02	0.19	0.00	0.00	0.00	0.11	0.01
2	6	-0.05	-0.13	-0.02	-0.11	0.13	-0.01	-0.04	-0.15	-0.01
3	6	0.17	0.08	0.01	0.01	-0.12	0.02	0.19	0.09	0.00
4	6	-0.17	0.08	0.01	0.01	0.12	-0.02	-0.19	0.09	0.00
5	6	0.05	-0.13	-0.02	-0.11	-0.13	0.01	0.04	-0.15	-0.01
6	1	-0.16	0.18	0.03	0.03	-0.30	0.02	-0.16	0.17	0.03
7	1	-0.26	-0.24	-0.01	0.16	-0.02	-0.04	-0.25	-0.23	-0.01
8	1	0.26	-0.24	-0.01	0.16	0.02	0.04	0.25	-0.23	-0.01
9	1	0.16	0.18	0.03	0.03	0.30	-0.02	0.16	0.17	0.03
10	1	0.00	0.12	-0.04	-0.37	0.00	-0.00	0.00	0.12	-0.03
11	6	-0.00	-0.11	0.02	-0.19	0.00	-0.00	0.00	0.11	-0.01
12	6	0.05	0.13	-0.02	0.11	-0.13	-0.01	-0.04	-0.15	0.01
13	6	-0.17	-0.08	0.01	-0.01	0.12	0.02	0.19	0.09	-0.00
14	6	0.17	-0.08	0.01	-0.01	-0.12	-0.02	-0.19	0.09	-0.00
15	6	-0.05	0.13	-0.02	0.11	0.13	0.01	0.04	-0.15	0.01
16	1	0.00	-0.12	-0.04	0.37	0.00	0.00	-0.00	0.12	0.03
17	1	0.16	-0.18	0.03	-0.03	0.30	0.02	-0.16	0.17	-0.03
18	1	0.26	0.24	-0.01	-0.16	0.02	-0.04	-0.25	-0.23	0.01
19	1	-0.26	0.24	-0.01	-0.16	-0.02	0.04	0.25	-0.23	0.01

20	1	-0.16	-0.18	0.03	-0.03	-0.30	-0.02	0.16	0.17	-0.03
21	44	0.00	0.00	-0.00	-0.00	-0.00	-0.00	-0.00	0.00	0.00

	43	44	45
	E2'	E1'	E1'
Frequencies --	1365.9906	1438.6717	1438.6721
Red. masses --	4.2184	2.1424	2.1424
Frc consts --	4.6376	2.6126	2.6126
IR Inten --	0.0000	7.5484	7.5466

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.22	0.00	0.00	0.00	0.08	0.01	-0.12	-0.00	-0.00
2	6	-0.11	0.15	-0.01	0.06	-0.10	0.00	0.06	0.06	0.01
3	6	0.01	-0.12	0.01	-0.09	0.01	-0.00	-0.05	-0.09	0.00
4	6	0.01	0.12	-0.01	0.09	0.01	-0.00	-0.05	0.09	-0.00
5	6	-0.11	-0.15	0.01	-0.06	-0.10	0.00	0.06	-0.06	-0.01
6	1	0.02	-0.30	0.02	-0.09	0.38	-0.00	0.13	-0.09	-0.00
7	1	0.16	-0.03	-0.03	0.15	0.21	0.00	0.30	0.15	-0.00
8	1	0.16	0.03	0.03	-0.15	0.21	0.00	0.30	-0.15	0.00
9	1	0.02	0.30	-0.02	0.09	0.38	-0.00	0.13	0.09	0.00
10	1	-0.36	0.00	-0.00	-0.00	0.10	-0.00	0.41	-0.00	0.00
11	6	0.22	-0.00	0.00	-0.00	0.08	-0.01	-0.12	0.00	-0.00
12	6	-0.11	0.15	0.01	0.06	-0.10	-0.00	0.06	0.06	-0.01
13	6	0.01	-0.12	-0.01	-0.09	0.01	0.00	-0.05	-0.09	-0.00
14	6	0.01	0.12	0.01	0.09	0.01	0.00	-0.05	0.09	0.00
15	6	-0.11	-0.15	-0.01	-0.06	-0.10	-0.00	0.06	-0.06	0.01
16	1	-0.36	-0.00	-0.00	0.00	0.10	0.00	0.41	0.00	0.00
17	1	0.02	-0.30	-0.02	-0.09	0.38	0.00	0.13	-0.09	0.00
18	1	0.16	-0.03	0.03	0.15	0.21	-0.00	0.30	0.15	0.00
19	1	0.16	0.03	-0.03	-0.15	0.21	-0.00	0.30	-0.15	-0.00
20	1	0.02	0.30	0.02	0.09	0.38	0.00	0.13	0.09	-0.00
21	44	0.00	0.00	0.00	-0.00	-0.00	0.00	-0.00	0.00	0.00

	46	47	48
	E1"	E1"	E2"
Frequencies --	1439.0429	1439.0434	3258.3279
Red. masses --	2.1220	2.1220	1.0890
Frc consts --	2.5891	2.5891	6.8121
IR Inten --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.00	0.08	0.01	-0.12	0.00	0.00	-0.00	0.00	0.00
2	6	0.06	-0.10	0.00	0.06	0.06	0.01	0.02	0.01	0.00
3	6	-0.09	0.01	-0.00	-0.05	-0.09	0.00	-0.02	0.03	-0.00
4	6	0.09	0.01	-0.00	-0.05	0.09	-0.00	-0.02	-0.03	0.00
5	6	-0.06	-0.10	0.00	0.06	-0.06	-0.01	0.02	-0.01	-0.00
6	1	-0.09	0.38	-0.00	0.13	-0.09	-0.01	-0.25	-0.08	-0.01
7	1	0.15	0.21	0.00	0.30	0.15	-0.00	0.25	-0.34	0.02
8	1	-0.15	0.20	0.00	0.30	-0.15	0.00	0.25	0.34	-0.02
9	1	0.09	0.38	-0.00	0.13	0.09	0.01	-0.25	0.08	0.01
10	1	0.00	0.10	-0.01	0.41	0.00	-0.00	0.00	-0.00	-0.00
11	6	-0.00	-0.08	0.01	0.12	0.00	-0.00	0.00	0.00	-0.00
12	6	-0.06	0.10	0.00	-0.06	-0.06	0.01	-0.02	-0.01	0.00
13	6	0.09	-0.01	-0.00	0.05	0.09	0.00	0.02	-0.03	-0.00

14	6	-0.09	-0.01	-0.00	0.05	-0.09	-0.00	0.02	0.03	0.00
15	6	0.06	0.10	0.00	-0.06	0.06	-0.01	-0.02	0.01	-0.00
16	1	0.00	-0.10	-0.01	-0.41	0.00	0.00	-0.00	-0.00	0.00
17	1	0.09	-0.38	-0.00	-0.13	0.09	-0.01	0.25	0.08	-0.01
18	1	-0.15	-0.20	0.00	-0.30	-0.15	-0.00	-0.25	0.34	0.02
19	1	0.15	-0.21	0.00	-0.30	0.15	0.00	-0.25	-0.34	-0.02
20	1	-0.09	-0.38	-0.00	-0.13	-0.09	0.01	0.25	-0.08	0.01
21	44	-0.00	-0.00	0.00	0.00	-0.00	0.00	-0.00	0.00	0.00

	49	50	51
	E2"	E2'	E2'
Frequencies --	3258.3280	3259.1539	3259.1540
Red. masses --	1.0890	1.0896	1.0896
Frc consts --	6.8121	6.8194	6.8194
IR Inten --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	-0.04	-0.00	0.00	0.00	0.00	-0.00	-0.04	-0.00
2	6	0.03	0.01	0.00	-0.02	-0.01	-0.00	0.03	0.01	0.00
3	6	-0.01	0.01	-0.00	0.02	-0.03	0.00	-0.01	0.01	-0.00
4	6	0.01	0.01	-0.00	0.02	0.03	-0.00	0.01	0.01	-0.00
5	6	-0.03	0.01	0.00	-0.02	0.01	0.00	-0.03	0.01	0.00
6	1	-0.34	-0.11	-0.02	0.25	0.08	0.01	-0.34	-0.11	-0.02
7	1	0.08	-0.11	0.01	-0.25	0.34	-0.02	0.08	-0.11	0.01
8	1	-0.08	-0.11	0.01	-0.25	-0.34	0.02	-0.08	-0.11	0.01
9	1	0.34	-0.11	-0.02	0.25	-0.08	-0.01	0.34	-0.11	-0.02
10	1	-0.00	0.45	0.02	-0.00	-0.00	-0.00	0.00	0.45	0.02
11	6	0.00	0.04	-0.00	0.00	-0.00	0.00	0.00	-0.04	0.00
12	6	-0.03	-0.01	0.00	-0.02	-0.01	0.00	0.03	0.01	-0.00
13	6	0.01	-0.01	-0.00	0.02	-0.03	-0.00	-0.01	0.01	0.00
14	6	-0.01	-0.01	-0.00	0.02	0.03	0.00	0.01	0.01	0.00
15	6	0.03	-0.01	0.00	-0.02	0.01	-0.00	-0.03	0.01	-0.00
16	1	-0.00	-0.45	0.02	-0.00	0.00	-0.00	-0.00	0.45	-0.02
17	1	0.34	0.11	-0.02	0.25	0.08	-0.01	-0.34	-0.11	0.02
18	1	-0.08	0.11	0.01	-0.25	0.34	0.02	0.08	-0.11	-0.01
19	1	0.08	0.11	0.01	-0.25	-0.34	-0.02	-0.08	-0.11	-0.01
20	1	-0.34	0.11	-0.02	0.25	-0.08	0.01	0.34	-0.11	0.02
21	44	-0.00	-0.00	0.00	0.00	0.00	-0.00	-0.00	-0.00	0.00

	52	53	54
	E1"	E1"	E1'
Frequencies --	3273.9850	3273.9853	3274.3424
Red. masses --	1.0953	1.0953	1.0957
Frc consts --	6.9170	6.9170	6.9210
IR Inten --	0.0000	0.0000	10.6545

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.00	-0.04	-0.00	0.00	0.00	0.00	0.00	-0.04	-0.00
2	6	-0.01	-0.00	-0.00	-0.04	-0.01	-0.00	-0.01	-0.00	-0.00
3	6	0.02	-0.03	0.00	-0.01	0.02	-0.00	0.02	-0.03	0.00
4	6	-0.02	-0.03	0.00	-0.01	-0.02	0.00	-0.02	-0.03	0.00
5	6	0.01	-0.00	-0.00	-0.04	0.01	0.00	0.01	-0.00	-0.00
6	1	0.13	0.04	0.01	0.40	0.13	0.02	0.13	0.04	0.01
7	1	-0.21	0.29	-0.02	0.15	-0.21	0.01	-0.21	0.29	-0.02

8	1	0.21	0.29	-0.02	0.15	0.21	-0.01	0.21	0.29	-0.02
9	1	-0.13	0.04	0.01	0.40	-0.13	-0.02	-0.13	0.04	0.01
10	1	0.00	0.45	0.02	-0.00	-0.00	-0.00	-0.00	0.45	0.02
11	6	-0.00	0.04	-0.00	-0.00	0.00	-0.00	-0.00	-0.04	0.00
12	6	0.01	0.00	-0.00	0.04	0.01	-0.00	-0.01	-0.00	0.00
13	6	-0.02	0.03	0.00	0.01	-0.02	-0.00	0.02	-0.03	-0.00
14	6	0.02	0.03	0.00	0.01	0.02	0.00	-0.02	-0.03	-0.00
15	6	-0.01	0.00	-0.00	0.04	-0.01	0.00	0.01	-0.00	0.00
16	1	0.00	-0.45	0.02	0.00	-0.00	0.00	0.00	0.45	-0.02
17	1	-0.13	-0.04	0.01	-0.40	-0.13	0.02	0.13	0.04	-0.01
18	1	0.21	-0.29	-0.02	-0.15	0.21	0.01	-0.21	0.29	0.02
19	1	-0.21	-0.29	-0.02	-0.15	-0.21	-0.01	0.21	0.29	0.02
20	1	0.13	-0.04	0.01	-0.40	0.13	-0.02	-0.13	0.04	-0.01
21	44	-0.00	-0.00	0.00	0.00	-0.00	0.00	-0.00	0.00	-0.00

	55	56	57
	E1'	A1'	A2"
Frequencies --	3274.3426	3290.6694	3291.0954
Red. masses --	1.0957	1.1067	1.1072
Frc consts --	6.9210	7.0609	7.0656
IR Inten --	10.6527	0.0000	3.3055

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	-0.00	-0.00	-0.00	-0.03	-0.00	0.00	-0.03	-0.00
2	6	-0.04	-0.01	-0.00	-0.03	-0.01	-0.00	-0.03	-0.01	-0.00
3	6	-0.01	0.02	-0.00	-0.02	0.02	-0.00	-0.02	0.02	-0.00
4	6	-0.01	-0.02	0.00	0.02	0.02	-0.00	0.02	0.02	-0.00
5	6	-0.04	0.01	0.00	0.03	-0.01	-0.00	0.03	-0.01	-0.00
6	1	0.40	0.13	0.02	0.30	0.10	0.01	0.30	0.10	0.01
7	1	0.15	-0.21	0.01	0.18	-0.25	0.01	0.18	-0.25	0.01
8	1	0.15	0.21	-0.01	-0.18	-0.25	0.01	-0.18	-0.25	0.01
9	1	0.40	-0.13	-0.02	-0.30	0.10	0.01	-0.30	0.10	0.01
10	1	-0.00	0.00	0.00	0.00	0.31	0.01	0.00	0.31	0.01
11	6	0.00	0.00	-0.00	0.00	-0.03	0.00	0.00	0.03	-0.00
12	6	-0.04	-0.01	0.00	-0.03	-0.01	0.00	0.03	0.01	-0.00
13	6	-0.01	0.02	0.00	-0.02	0.02	0.00	0.02	-0.02	-0.00
14	6	-0.01	-0.02	-0.00	0.02	0.02	0.00	-0.02	-0.02	-0.00
15	6	-0.04	0.01	-0.00	0.03	-0.01	0.00	-0.03	0.01	-0.00
16	1	-0.00	-0.00	0.00	-0.00	0.31	-0.01	0.00	-0.31	0.01
17	1	0.40	0.13	-0.02	0.30	0.10	-0.01	-0.30	-0.10	0.01
18	1	0.15	-0.21	-0.01	0.18	-0.25	-0.01	-0.18	0.25	0.01
19	1	0.15	0.21	0.01	-0.18	-0.25	-0.01	0.18	0.25	0.01
20	1	0.40	-0.13	0.02	-0.30	0.10	-0.01	0.30	-0.10	0.01
21	44	0.00	0.00	0.00	-0.00	-0.00	0.00	0.00	-0.00	0.00

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Atom 1 has atomic number 6 and mass 12.00000
Atom 2 has atomic number 6 and mass 12.00000
Atom 3 has atomic number 6 and mass 12.00000

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Atom     4 has atomic number  6 and mass  12.00000
Atom     5 has atomic number  6 and mass  12.00000
Atom     6 has atomic number  1 and mass   1.00783
Atom     7 has atomic number  1 and mass   1.00783
Atom     8 has atomic number  1 and mass   1.00783
Atom     9 has atomic number  1 and mass   1.00783
Atom    10 has atomic number  1 and mass   1.00783
Atom    11 has atomic number  6 and mass  12.00000
Atom    12 has atomic number  6 and mass  12.00000
Atom    13 has atomic number  6 and mass  12.00000
Atom    14 has atomic number  6 and mass  12.00000
Atom    15 has atomic number  6 and mass  12.00000
Atom    16 has atomic number  1 and mass   1.00783
Atom    17 has atomic number  1 and mass   1.00783
Atom    18 has atomic number  1 and mass   1.00783
Atom    19 has atomic number  1 and mass   1.00783
Atom    20 has atomic number  1 and mass   1.00783
Atom    21 has atomic number 44 and mass 101.90370
Molecular mass:   231.98195 amu.
Principal axes and moments of inertia in atomic units:
                          1         2         3
    Eigenvalues --   833.83349 2070.65255 2070.65255
          X            0.00000   1.00000   0.00000
          Y            0.00000   0.00000   1.00000
          Z            1.00000   0.00000   0.00000
This molecule is a prolate symmetric top.
Rotational symmetry number 10.
Warning -- assumption of classical behavior for rotation
          may cause significant error
Rotational temperatures (Kelvin)      0.10387     0.04183     0.04183
Rotational constants (GHZ):           2.16439     0.87158     0.87158
Zero-point vibrational energy     441822.8 (Joules/Mol)
                                  105.59818 (Kcal/Mol)
Warning -- explicit consideration of  13 degrees of freedom as
          vibrations may cause significant error
Vibrational temperatures:     56.30   208.99   208.99   442.91   511.40
         (Kelvin)            511.40   540.95   606.62   606.62   816.13
                             816.13   836.27   836.27  1157.23  1159.13
                            1159.13  1173.87  1205.98  1205.98  1213.87
                            1213.87  1247.41  1247.41  1255.84  1255.84
                            1275.03  1275.03  1453.36  1453.36  1465.72
                            1465.72  1559.97  1559.97  1577.14  1577.14
                            1596.74  1603.67  1887.89  1888.01  1933.06
                            1933.06  1965.36  1965.36  2069.93  2069.93
                            2070.46  2070.46  4688.01  4688.01  4689.20
                            4689.20  4710.53  4710.53  4711.05  4711.05
                            4734.54  4735.15

Zero-point correction=                           0.168281 (Hartree/Particle)
Thermal correction to Energy=                    0.177309
```

Thermal correction to Enthalpy= 0.178254
Thermal correction to Gibbs Free Energy= 0.135531
Sum of electronic and zero-point Energies= -4808.037502
Sum of electronic and thermal Energies= -4808.028474
Sum of electronic and thermal Enthalpies= -4808.027530
Sum of electronic and thermal Free Energies= -4808.070253

		E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total		111.263	37.653	89.917
Electronic		0.000	0.000	0.000
Translational		0.889	2.981	42.226
Rotational		0.889	2.981	25.084
Vibrational		109.486	31.691	22.607
Vibration	1	0.594	1.981	5.303
Vibration	2	0.617	1.908	2.733
Vibration	3	0.617	1.908	2.733
Vibration	4	0.698	1.659	1.374
Vibration	5	0.731	1.564	1.142
Vibration	6	0.731	1.564	1.142
Vibration	7	0.747	1.521	1.055
Vibration	8	0.784	1.423	0.886
Vibration	9	0.784	1.423	0.886
Vibration	10	0.923	1.102	0.510
Vibration	11	0.923	1.102	0.510
Vibration	12	0.938	1.072	0.483
Vibration	13	0.938	1.072	0.483

		Q	Log10(Q)	Ln(Q)
Total Bot		0.457110D-62	-62.339979	-143.543106
Total V=0		0.115886D+16	15.064029	34.686209
Vib (Bot)		0.486288D-75	-75.313107	-173.414836
Vib (Bot)	1	0.528790D+01	0.723283	1.665420
Vib (Bot)	2	0.139782D+01	0.145453	0.334917
Vib (Bot)	3	0.139781D+01	0.145448	0.334907
Vib (Bot)	4	0.615031D+00	-0.211103	-0.486082
Vib (Bot)	5	0.517231D+00	-0.286316	-0.659266
Vib (Bot)	6	0.517230D+00	-0.286316	-0.659267
Vib (Bot)	7	0.482242D+00	-0.316735	-0.729309
Vib (Bot)	8	0.415948D+00	-0.380961	-0.877195
Vib (Bot)	9	0.415947D+00	-0.380962	-0.877196
Vib (Bot)	10	0.272064D+00	-0.565330	-1.301719
Vib (Bot)	11	0.272063D+00	-0.565330	-1.301720
Vib (Bot)	12	0.261844D+00	-0.581958	-1.340007
Vib (Bot)	13	0.261844D+00	-0.581958	-1.340008
Vib (V=0)		0.123283D+03	2.090902	4.814479
Vib (V=0)	1	0.581148D+01	0.764287	1.759836
Vib (V=0)	2	0.198456D+01	0.297664	0.685396
Vib (V=0)	3	0.198454D+01	0.297661	0.685390
Vib (V=0)	4	0.129263D+01	0.111475	0.256680
Vib (V=0)	5	0.121939D+01	0.086144	0.198354

```
Vib (V=0)    6  0.121939D+01          0.086144          0.198354
Vib (V=0)    7  0.119466D+01          0.077246          0.177865
Vib (V=0)    8  0.115039D+01          0.060847          0.140105
Vib (V=0)    9  0.115039D+01          0.060847          0.140104
Vib (V=0)   10  0.106923D+01          0.029070          0.066935
Vib (V=0)   11  0.106923D+01          0.029070          0.066935
Vib (V=0)   12  0.106441D+01          0.027110          0.062424
Vib (V=0)   13  0.106441D+01          0.027110          0.062423
Electronic      0.100000D+01          0.000000          0.000000
Translational   0.138879D+09          8.142635         18.749110
Rotational      0.676850D+05          4.830492         11.122620
***** Axes restored to original set *****
-------------------------------------------------------------------
Center     Atomic                   Forces (Hartrees/Bohr)
Number     Number              X              Y              Z
-------------------------------------------------------------------
     1        6           0.000000000   -0.000004883   -0.000000098
     2        6           0.000004644   -0.000001509   -0.000000098
     3        6           0.000002870    0.000003950   -0.000000098
     4        6          -0.000002870    0.000003950   -0.000000098
     5        6          -0.000004644   -0.000001509   -0.000000098
     6        1           0.000008842   -0.000002873    0.000000995
     7        1           0.000005465    0.000007521    0.000000995
     8        1          -0.000005465    0.000007521    0.000000995
     9        1          -0.000008842   -0.000002873    0.000000995
    10        1           0.000000000   -0.000009297    0.000000995
    11        6           0.000000000   -0.000004883    0.000000098
    12        6           0.000004644   -0.000001509    0.000000098
    13        6           0.000002870    0.000003950    0.000000098
    14        6          -0.000002870    0.000003950    0.000000098
    15        6          -0.000004644   -0.000001509    0.000000098
    16        1          -0.000000000   -0.000009297   -0.000000995
    17        1           0.000008842   -0.000002873   -0.000000995
    18        1           0.000005465    0.000007521   -0.000000995
    19        1          -0.000005465    0.000007521   -0.000000995
    20        1          -0.000008842   -0.000002873   -0.000000995
    21       44           0.000000000    0.000000000   -0.000000000
-------------------------------------------------------------------
Cartesian Forces:  Max     0.000009297 RMS     0.000004203
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Internal  Forces:  Max     0.000009329 RMS     0.000002940
Search for a local minimum.
Step number   1 out of a maximum of    2
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Second derivative matrix not updated -- analytic derivatives used.
ITU=  0
    Eigenvalues ---    0.00070   0.00221   0.00221   0.01020   0.01020
```

```
    Eigenvalues ---    0.01050   0.01050   0.01261   0.01261   0.01306
    Eigenvalues ---    0.01306   0.01343   0.01343   0.01454   0.01454
    Eigenvalues ---    0.01477   0.01679   0.01750   0.01750   0.02051
    Eigenvalues ---    0.02051   0.02306   0.02362   0.03086   0.03424
    Eigenvalues ---    0.03424   0.03713   0.03713   0.05689   0.06880
    Eigenvalues ---    0.06880   0.07357   0.07357   0.11771   0.11771
    Eigenvalues ---    0.14135   0.14135   0.19669   0.20976   0.20976
    Eigenvalues ---    0.21602   0.21602   0.23064   0.23064   0.26142
    Eigenvalues ---    0.26142   0.30221   0.37568   0.37568   0.37594
    Eigenvalues ---    0.37594   0.37631   0.37631   0.37640   0.37640
    Eigenvalues ---    0.37726   0.37732
Angle between quadratic step and forces=  28.43 degrees.
Linear search not attempted -- first point.
Iteration  1 RMS(Cart)=  0.00001254 RMS(Int)=  0.00000000
Iteration  2 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000000
ClnCor:  largest displacement from symmetrization is 1.67D-08 for atom     7.
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                (Linear)    (Quad)   (Total)
   R1        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
   R2        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
   R3        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
   R4        4.24579  -0.00000   0.00000  -0.00002  -0.00002   4.24577
   R5        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
   R6        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
   R7        4.24579  -0.00000   0.00000  -0.00002  -0.00002   4.24577
   R8        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
   R9        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
  R10        4.24579  -0.00000   0.00000  -0.00002  -0.00002   4.24577
  R11        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
  R12        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
  R13        4.24579  -0.00000   0.00000  -0.00002  -0.00002   4.24577
  R14        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
  R15        4.24579  -0.00000   0.00000  -0.00002  -0.00002   4.24577
  R16        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
  R17        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
  R18        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
  R19        4.24579  -0.00000   0.00000  -0.00002  -0.00002   4.24577
  R20        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
  R21        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
  R22        4.24579  -0.00000   0.00000  -0.00002  -0.00002   4.24577
  R23        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
  R24        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
  R25        4.24579  -0.00000   0.00000  -0.00002  -0.00002   4.24577
  R26        2.72129  -0.00001   0.00000  -0.00003  -0.00003   2.72126
  R27        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
  R28        4.24579  -0.00000   0.00000  -0.00002  -0.00002   4.24577
  R29        2.03784  -0.00001   0.00000  -0.00002  -0.00002   2.03782
  R30        4.24579  -0.00000   0.00000  -0.00002  -0.00002   4.24577
   A1        1.88496   0.00000   0.00000  -0.00000   0.00000   1.88496
   A2        2.19854  -0.00000   0.00000   0.00000   0.00000   2.19854
```

A3	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A4	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A5	1.88496	0.00000	0.00000	-0.00000	0.00000	1.88496
A6	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A7	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A8	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A9	1.88496	-0.00000	0.00000	0.00000	0.00000	1.88496
A10	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A11	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A12	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A13	1.88496	-0.00000	0.00000	0.00000	-0.00000	1.88496
A14	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A15	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A16	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A17	1.88496	0.00000	0.00000	-0.00000	0.00000	1.88496
A18	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A19	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A20	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A21	1.88496	0.00000	0.00000	-0.00000	0.00000	1.88496
A22	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A23	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A24	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A25	1.88496	-0.00000	0.00000	-0.00000	-0.00000	1.88496
A26	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A27	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A28	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A29	1.88496	-0.00000	0.00000	0.00000	0.00000	1.88496
A30	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A31	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A32	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A33	1.88496	0.00000	0.00000	0.00000	-0.00000	1.88496
A34	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A35	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A36	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A37	1.88496	-0.00000	0.00000	-0.00000	0.00000	1.88496
A38	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A39	2.19854	-0.00000	0.00000	0.00000	0.00000	2.19854
A40	2.18729	-0.00000	0.00000	-0.00001	-0.00001	2.18728
A41	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A42	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A43	1.98830	0.00000	0.00000	0.00001	0.00001	1.98831
A44	2.22797	0.00000	0.00000	0.00001	0.00001	2.22798
A45	2.80302	0.00000	0.00000	0.00000	0.00000	2.80302
A46	2.80302	0.00000	0.00000	0.00000	0.00000	2.80302
A47	2.22797	0.00000	0.00000	0.00001	0.00001	2.22798
A48	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A49	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A50	2.22797	0.00000	0.00000	0.00001	0.00001	2.22798
A51	1.98830	0.00000	0.00000	0.00001	0.00001	1.98831
A52	2.22797	0.00000	0.00000	0.00001	0.00001	2.22798

A53	2.80302	0.00000	0.00000	0.00000	0.00000	2.80302
A54	2.80302	0.00000	0.00000	0.00000	0.00000	2.80302
A55	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A56	2.80302	0.00000	0.00000	0.00000	0.00000	2.80302
A57	2.22797	0.00000	0.00000	0.00001	0.00001	2.22798
A58	1.98830	0.00000	0.00000	0.00001	0.00001	1.98831
A59	2.22797	0.00000	0.00000	0.00001	0.00001	2.22798
A60	2.80302	0.00000	0.00000	0.00000	0.00000	2.80302
A61	2.80302	0.00000	0.00000	0.00000	0.00000	2.80302
A62	2.80302	0.00000	0.00000	0.00000	0.00000	2.80302
A63	2.22797	0.00000	0.00000	0.00001	0.00001	2.22798
A64	1.98830	0.00000	0.00000	0.00001	0.00001	1.98831
A65	2.22797	0.00000	0.00000	0.00001	0.00001	2.22798
A66	2.22797	0.00000	0.00000	0.00001	0.00001	2.22798
A67	2.80302	0.00000	0.00000	0.00000	0.00000	2.80302
A68	2.80302	0.00000	0.00000	0.00000	0.00000	2.80302
A69	2.22797	0.00000	0.00000	0.00001	0.00001	2.22798
A70	1.98830	0.00000	0.00000	0.00001	0.00001	1.98831
A71	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A72	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A73	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A74	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
A75	1.09026	-0.00000	0.00000	-0.00001	-0.00001	1.09025
D1	0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
D2	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09236
D3	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09236
D4	0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
D5	0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
D6	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09236
D7	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09236
D8	-0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
D9	2.77183	0.00000	0.00000	0.00000	0.00000	2.77183
D10	-2.77183	-0.00000	0.00000	-0.00000	-0.00000	-2.77183
D11	-0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
D12	0.71410	-0.00000	0.00000	-0.00000	-0.00000	0.71410
D13	1.30487	-0.00000	0.00000	-0.00000	-0.00000	1.30487
D14	-1.30487	0.00000	0.00000	0.00000	0.00000	-1.30487
D15	-0.71410	0.00000	0.00000	0.00000	0.00000	-0.71410
D16	0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
D17	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09236
D18	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09236
D19	0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
D20	2.77183	0.00000	0.00000	0.00000	0.00000	2.77183
D21	-2.77183	-0.00000	0.00000	-0.00000	-0.00000	-2.77183
D22	-0.71410	0.00000	0.00000	0.00000	0.00000	-0.71410
D23	-0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
D24	0.71410	-0.00000	0.00000	-0.00000	-0.00000	0.71410
D25	1.30487	-0.00000	0.00000	-0.00000	-0.00000	1.30487
D26	-1.30487	0.00000	0.00000	0.00000	0.00000	-1.30487
D27	0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000

D28	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09236
D29	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09236
D30	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D31	-2.77183	-0.00000	0.00000	-0.00000	-0.00000	-2.77183
D32	2.77183	0.00000	0.00000	0.00000	0.00000	2.77183
D33	-1.30487	0.00000	0.00000	0.00000	0.00000	-1.30487
D34	-0.71410	0.00000	0.00000	0.00000	0.00000	-0.71410
D35	-0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
D36	0.71410	-0.00000	0.00000	-0.00000	-0.00000	0.71410
D37	1.30487	-0.00000	0.00000	-0.00000	-0.00000	1.30487
D38	0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
D39	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09236
D40	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09236
D41	0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
D42	2.77183	0.00000	0.00000	0.00000	0.00000	2.77183
D43	-2.77183	-0.00000	0.00000	-0.00000	-0.00000	-2.77183
D44	1.30487	-0.00000	0.00000	-0.00000	-0.00000	1.30487
D45	-1.30487	0.00000	0.00000	0.00000	0.00000	-1.30487
D46	-0.71410	0.00000	0.00000	0.00000	0.00000	-0.71410
D47	-0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
D48	0.71410	-0.00000	0.00000	-0.00000	-0.00000	0.71410
D49	2.77183	0.00000	0.00000	0.00000	0.00000	2.77183
D50	-2.77183	-0.00000	0.00000	-0.00000	-0.00000	-2.77183
D51	0.71410	-0.00000	0.00000	-0.00000	-0.00000	0.71410
D52	1.30487	-0.00000	0.00000	-0.00000	-0.00000	1.30487
D53	-1.30487	0.00000	0.00000	0.00000	0.00000	-1.30487
D54	-0.71410	0.00000	0.00000	0.00000	0.00000	-0.71410
D55	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000
D56	-0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
D57	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09236
D58	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09236
D59	-0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
D60	-0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
D61	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09236
D62	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09236
D63	0.00000	-0.00000	0.00000	0.00000	0.00000	0.00000
D64	-0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
D65	-0.71410	0.00000	0.00000	0.00000	0.00000	-0.71410
D66	-1.30487	0.00000	0.00000	0.00000	0.00000	-1.30487
D67	1.30487	-0.00000	0.00000	-0.00000	-0.00000	1.30487
D68	0.71410	-0.00000	0.00000	-0.00000	-0.00000	0.71410
D69	-2.77183	-0.00000	0.00000	-0.00000	-0.00000	-2.77183
D70	2.77183	0.00000	0.00000	0.00000	0.00000	2.77183
D71	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00000
D72	3.09235	-0.00000	0.00000	0.00001	0.00001	3.09236
D73	-3.09235	0.00000	0.00000	-0.00001	-0.00001	-3.09236
D74	-0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
D75	0.71410	-0.00000	0.00000	-0.00000	-0.00000	0.71410
D76	0.00000	0.00000	0.00000	-0.00000	0.00000	0.00000
D77	-0.71410	0.00000	0.00000	0.00000	0.00000	-0.71410

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  D78       -1.30487   0.00000   0.00000   0.00000   0.00000  -1.30487
  D79        1.30487  -0.00000   0.00000  -0.00000  -0.00000   1.30487
  D80       -2.77183  -0.00000   0.00000  -0.00000  -0.00000  -2.77183
  D81        2.77183   0.00000   0.00000   0.00000   0.00000   2.77183
  D82       -0.00000   0.00000   0.00000  -0.00000   0.00000   0.00000
  D83        3.09235  -0.00000   0.00000   0.00001   0.00001   3.09236
  D84       -3.09235   0.00000   0.00000  -0.00001  -0.00001  -3.09236
  D85        0.00000  -0.00000   0.00000   0.00000   0.00000   0.00000
  D86        1.30487  -0.00000   0.00000  -0.00000  -0.00000   1.30487
  D87        0.71410  -0.00000   0.00000  -0.00000  -0.00000   0.71410
  D88       -0.00000   0.00000   0.00000  -0.00000  -0.00000  -0.00000
  D89       -0.71410   0.00000   0.00000   0.00000   0.00000  -0.71410
  D90       -1.30487   0.00000   0.00000   0.00000   0.00000  -1.30487
  D91        2.77183   0.00000   0.00000   0.00000   0.00000   2.77183
  D92       -2.77183  -0.00000   0.00000  -0.00000  -0.00000  -2.77183
  D93        0.00000  -0.00000   0.00000   0.00000   0.00000   0.00000
  D94        3.09235  -0.00000   0.00000   0.00001   0.00001   3.09236
  D95       -3.09235   0.00000   0.00000  -0.00001  -0.00001  -3.09236
  D96       -0.00000   0.00000   0.00000  -0.00000   0.00000   0.00000
  D97       -1.30487   0.00000   0.00000   0.00000   0.00000  -1.30487
  D98        1.30487  -0.00000   0.00000  -0.00000  -0.00000   1.30487
  D99        0.71410  -0.00000   0.00000  -0.00000  -0.00000   0.71410
  D100       0.00000   0.00000   0.00000  -0.00000   0.00000   0.00000
  D101      -0.71410   0.00000   0.00000   0.00000   0.00000  -0.71410
  D102      -2.77183  -0.00000   0.00000  -0.00000  -0.00000  -2.77183
  D103       2.77183   0.00000   0.00000   0.00000   0.00000   2.77183
  D104      -0.71410   0.00000   0.00000   0.00000   0.00000  -0.71410
  D105      -1.30487   0.00000   0.00000   0.00000   0.00000  -1.30487
  D106       1.30487  -0.00000   0.00000  -0.00000  -0.00000   1.30487
  D107       0.71410  -0.00000   0.00000  -0.00000  -0.00000   0.71410
  D108      -0.00000   0.00000   0.00000  -0.00000   0.00000   0.00000
  D109      -2.77183  -0.00000   0.00000  -0.00000  -0.00000  -2.77183
  D110       2.77183   0.00000   0.00000   0.00000   0.00000   2.77183
         Item               Value     Threshold  Converged?
Maximum Force            0.000009     0.000450     YES
RMS     Force            0.000003     0.000300     YES
Maximum Displacement     0.000046     0.001800     YES
RMS     Displacement     0.000013     0.001200     YES
Predicted change in Energy=-2.845789D-09
Optimization completed.
   -- Stationary point found.
                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
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! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.44           -DE/DX =    0.0                 !
! R2    R(1,5)                  1.44           -DE/DX =    0.0                 !
! R3    R(1,10)                 1.0784         -DE/DX =    0.0                 !
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! R4    R(1,21)              2.2468         -DE/DX =    0.0              !
! R5    R(2,3)               1.44           -DE/DX =    0.0              !
! R6    R(2,6)               1.0784         -DE/DX =    0.0              !
! R7    R(2,21)              2.2468         -DE/DX =    0.0              !
! R8    R(3,4)               1.44           -DE/DX =    0.0              !
! R9    R(3,7)               1.0784         -DE/DX =    0.0              !
! R10   R(3,21)              2.2468         -DE/DX =    0.0              !
! R11   R(4,5)               1.44           -DE/DX =    0.0              !
! R12   R(4,8)               1.0784         -DE/DX =    0.0              !
! R13   R(4,21)              2.2468         -DE/DX =    0.0              !
! R14   R(5,9)               1.0784         -DE/DX =    0.0              !
! R15   R(5,21)              2.2468         -DE/DX =    0.0              !
! R16   R(11,12)             1.44           -DE/DX =    0.0              !
! R17   R(11,15)             1.44           -DE/DX =    0.0              !
! R18   R(11,16)             1.0784         -DE/DX =    0.0              !
! R19   R(11,21)             2.2468         -DE/DX =    0.0              !
! R20   R(12,13)             1.44           -DE/DX =    0.0              !
! R21   R(12,17)             1.0784         -DE/DX =    0.0              !
! R22   R(12,21)             2.2468         -DE/DX =    0.0              !
! R23   R(13,14)             1.44           -DE/DX =    0.0              !
! R24   R(13,18)             1.0784         -DE/DX =    0.0              !
! R25   R(13,21)             2.2468         -DE/DX =    0.0              !
! R26   R(14,15)             1.44           -DE/DX =    0.0              !
! R27   R(14,19)             1.0784         -DE/DX =    0.0              !
! R28   R(14,21)             2.2468         -DE/DX =    0.0              !
! R29   R(15,20)             1.0784         -DE/DX =    0.0              !
! R30   R(15,21)             2.2468         -DE/DX =    0.0              !
! A1    A(2,1,5)           108.0            -DE/DX =    0.0              !
! A2    A(2,1,10)          125.967          -DE/DX =    0.0              !
! A3    A(5,1,10)          125.967          -DE/DX =    0.0              !
! A4    A(10,1,21)         125.3225         -DE/DX =    0.0              !
! A5    A(1,2,3)           108.0            -DE/DX =    0.0              !
! A6    A(1,2,6)           125.967          -DE/DX =    0.0              !
! A7    A(3,2,6)           125.967          -DE/DX =    0.0              !
! A8    A(6,2,21)          125.3225         -DE/DX =    0.0              !
! A9    A(2,3,4)           108.0            -DE/DX =    0.0              !
! A10   A(2,3,7)           125.967          -DE/DX =    0.0              !
! A11   A(4,3,7)           125.967          -DE/DX =    0.0              !
! A12   A(7,3,21)          125.3225         -DE/DX =    0.0              !
! A13   A(3,4,5)           108.0            -DE/DX =    0.0              !
! A14   A(3,4,8)           125.967          -DE/DX =    0.0              !
! A15   A(5,4,8)           125.967          -DE/DX =    0.0              !
! A16   A(8,4,21)          125.3225         -DE/DX =    0.0              !
! A17   A(1,5,4)           108.0            -DE/DX =    0.0              !
! A18   A(1,5,9)           125.967          -DE/DX =    0.0              !
! A19   A(4,5,9)           125.967          -DE/DX =    0.0              !
! A20   A(9,5,21)          125.3225         -DE/DX =    0.0              !
! A21   A(12,11,15)        108.0            -DE/DX =    0.0              !
! A22   A(12,11,16)        125.967          -DE/DX =    0.0              !
! A23   A(15,11,16)        125.967          -DE/DX =    0.0              !
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! A24   A(16,11,21)          125.3225         -DE/DX =    0.0               !
! A25   A(11,12,13)          108.0            -DE/DX =    0.0               !
! A26   A(11,12,17)          125.967          -DE/DX =    0.0               !
! A27   A(13,12,17)          125.967          -DE/DX =    0.0               !
! A28   A(17,12,21)          125.3225         -DE/DX =    0.0               !
! A29   A(12,13,14)          108.0            -DE/DX =    0.0               !
! A30   A(12,13,18)          125.967          -DE/DX =    0.0               !
! A31   A(14,13,18)          125.967          -DE/DX =    0.0               !
! A32   A(18,13,21)          125.3225         -DE/DX =    0.0               !
! A33   A(13,14,15)          108.0            -DE/DX =    0.0               !
! A34   A(13,14,19)          125.967          -DE/DX =    0.0               !
! A35   A(15,14,19)          125.967          -DE/DX =    0.0               !
! A36   A(19,14,21)          125.3225         -DE/DX =    0.0               !
! A37   A(11,15,14)          108.0            -DE/DX =    0.0               !
! A38   A(11,15,20)          125.967          -DE/DX =    0.0               !
! A39   A(14,15,20)          125.967          -DE/DX =    0.0               !
! A40   A(20,15,21)          125.3225         -DE/DX =    0.0               !
! A41   A(1,21,3)             62.4674         -DE/DX =    0.0               !
! A42   A(1,21,4)             62.4674         -DE/DX =    0.0               !
! A43   A(1,21,11)           113.9213         -DE/DX =    0.0               !
! A44   A(1,21,12)           127.6534         -DE/DX =    0.0               !
! A45   A(1,21,13)           160.601          -DE/DX =    0.0               !
! A46   A(1,21,14)           160.601          -DE/DX =    0.0               !
! A47   A(1,21,15)           127.6534         -DE/DX =    0.0               !
! A48   A(2,21,4)             62.4674         -DE/DX =    0.0               !
! A49   A(2,21,5)             62.4674         -DE/DX =    0.0               !
! A50   A(2,21,11)           127.6534         -DE/DX =    0.0               !
! A51   A(2,21,12)           113.9213         -DE/DX =    0.0               !
! A52   A(2,21,13)           127.6534         -DE/DX =    0.0               !
! A53   A(2,21,14)           160.601          -DE/DX =    0.0               !
! A54   A(2,21,15)           160.601          -DE/DX =    0.0               !
! A55   A(3,21,5)             62.4674         -DE/DX =    0.0               !
! A56   A(3,21,11)           160.601          -DE/DX =    0.0               !
! A57   A(3,21,12)           127.6534         -DE/DX =    0.0               !
! A58   A(3,21,13)           113.9213         -DE/DX =    0.0               !
! A59   A(3,21,14)           127.6534         -DE/DX =    0.0               !
! A60   A(3,21,15)           160.601          -DE/DX =    0.0               !
! A61   A(4,21,11)           160.601          -DE/DX =    0.0               !
! A62   A(4,21,12)           160.601          -DE/DX =    0.0               !
! A63   A(4,21,13)           127.6534         -DE/DX =    0.0               !
! A64   A(4,21,14)           113.9213         -DE/DX =    0.0               !
! A65   A(4,21,15)           127.6534         -DE/DX =    0.0               !
! A66   A(5,21,11)           127.6534         -DE/DX =    0.0               !
! A67   A(5,21,12)           160.601          -DE/DX =    0.0               !
! A68   A(5,21,13)           160.601          -DE/DX =    0.0               !
! A69   A(5,21,14)           127.6534         -DE/DX =    0.0               !
! A70   A(5,21,15)           113.9213         -DE/DX =    0.0               !
! A71   A(11,21,13)           62.4674         -DE/DX =    0.0               !
! A72   A(11,21,14)           62.4674         -DE/DX =    0.0               !
! A73   A(12,21,14)           62.4674         -DE/DX =    0.0               !
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! A74   A(12,21,15)           62.4674         -DE/DX =    0.0               !
! A75   A(13,21,15)           62.4674         -DE/DX =    0.0               !
! D1    D(5,1,2,3)              0.0           -DE/DX =    0.0               !
! D2    D(5,1,2,6)           -177.1787        -DE/DX =    0.0               !
! D3    D(10,1,2,3)           177.1787        -DE/DX =    0.0               !
! D4    D(10,1,2,6)             0.0           -DE/DX =    0.0               !
! D5    D(2,1,5,4)              0.0           -DE/DX =    0.0               !
! D6    D(2,1,5,9)            177.1787        -DE/DX =    0.0               !
! D7    D(10,1,5,4)          -177.1787        -DE/DX =    0.0               !
! D8    D(10,1,5,9)             0.0           -DE/DX =    0.0               !
! D9    D(10,1,21,3)          158.8139        -DE/DX =    0.0               !
! D10   D(10,1,21,4)         -158.8139        -DE/DX =    0.0               !
! D11   D(10,1,21,11)            0.0           -DE/DX =    0.0               !
! D12   D(10,1,21,12)           40.9151        -DE/DX =    0.0               !
! D13   D(10,1,21,13)           74.7635        -DE/DX =    0.0               !
! D14   D(10,1,21,14)          -74.7635        -DE/DX =    0.0               !
! D15   D(10,1,21,15)          -40.9151        -DE/DX =    0.0               !
! D16   D(1,2,3,4)               0.0           -DE/DX =    0.0               !
! D17   D(1,2,3,7)            -177.1787        -DE/DX =    0.0               !
! D18   D(6,2,3,4)             177.1787        -DE/DX =    0.0               !
! D19   D(6,2,3,7)               0.0           -DE/DX =    0.0               !
! D20   D(6,2,21,4)            158.8139        -DE/DX =    0.0               !
! D21   D(6,2,21,5)           -158.8139        -DE/DX =    0.0               !
! D22   D(6,2,21,11)           -40.9151        -DE/DX =    0.0               !
! D23   D(6,2,21,12)             0.0           -DE/DX =    0.0               !
! D24   D(6,2,21,13)            40.9151        -DE/DX =    0.0               !
! D25   D(6,2,21,14)            74.7635        -DE/DX =    0.0               !
! D26   D(6,2,21,15)           -74.7635        -DE/DX =    0.0               !
! D27   D(2,3,4,5)               0.0           -DE/DX =    0.0               !
! D28   D(2,3,4,8)            -177.1787        -DE/DX =    0.0               !
! D29   D(7,3,4,5)             177.1787        -DE/DX =    0.0               !
! D30   D(7,3,4,8)               0.0           -DE/DX =    0.0               !
! D31   D(7,3,21,1)           -158.8139        -DE/DX =    0.0               !
! D32   D(7,3,21,5)            158.8139        -DE/DX =    0.0               !
! D33   D(7,3,21,11)           -74.7635        -DE/DX =    0.0               !
! D34   D(7,3,21,12)           -40.9151        -DE/DX =    0.0               !
! D35   D(7,3,21,13)             0.0           -DE/DX =    0.0               !
! D36   D(7,3,21,14)            40.9151        -DE/DX =    0.0               !
! D37   D(7,3,21,15)            74.7635        -DE/DX =    0.0               !
! D38   D(3,4,5,1)               0.0           -DE/DX =    0.0               !
! D39   D(3,4,5,9)            -177.1787        -DE/DX =    0.0               !
! D40   D(8,4,5,1)             177.1787        -DE/DX =    0.0               !
! D41   D(8,4,5,9)               0.0           -DE/DX =    0.0               !
! D42   D(8,4,21,1)            158.8139        -DE/DX =    0.0               !
! D43   D(8,4,21,2)           -158.8139        -DE/DX =    0.0               !
! D44   D(8,4,21,11)            74.7635        -DE/DX =    0.0               !
! D45   D(8,4,21,12)           -74.7635        -DE/DX =    0.0               !
! D46   D(8,4,21,13)           -40.9151        -DE/DX =    0.0               !
! D47   D(8,4,21,14)             0.0           -DE/DX =    0.0               !
! D48   D(8,4,21,15)            40.9151        -DE/DX =    0.0               !
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! D49   D(9,5,21,2)          158.8139         -DE/DX =    0.0               !
! D50   D(9,5,21,3)         -158.8139         -DE/DX =    0.0               !
! D51   D(9,5,21,11)          40.9151         -DE/DX =    0.0               !
! D52   D(9,5,21,12)          74.7635         -DE/DX =    0.0               !
! D53   D(9,5,21,13)         -74.7635         -DE/DX =    0.0               !
! D54   D(9,5,21,14)         -40.9151         -DE/DX =    0.0               !
! D55   D(9,5,21,15)           0.0            -DE/DX =    0.0               !
! D56   D(15,11,12,13)         0.0            -DE/DX =    0.0               !
! D57   D(15,11,12,17)       177.1787         -DE/DX =    0.0               !
! D58   D(16,11,12,13)      -177.1787         -DE/DX =    0.0               !
! D59   D(16,11,12,17)         0.0            -DE/DX =    0.0               !
! D60   D(12,11,15,14)         0.0            -DE/DX =    0.0               !
! D61   D(12,11,15,20)      -177.1787         -DE/DX =    0.0               !
! D62   D(16,11,15,14)       177.1787         -DE/DX =    0.0               !
! D63   D(16,11,15,20)         0.0            -DE/DX =    0.0               !
! D64   D(16,11,21,1)          0.0            -DE/DX =    0.0               !
! D65   D(16,11,21,2)        -40.9151         -DE/DX =    0.0               !
! D66   D(16,11,21,3)        -74.7635         -DE/DX =    0.0               !
! D67   D(16,11,21,4)         74.7635         -DE/DX =    0.0               !
! D68   D(16,11,21,5)         40.9151         -DE/DX =    0.0               !
! D69   D(16,11,21,13)      -158.8139         -DE/DX =    0.0               !
! D70   D(16,11,21,14)       158.8139         -DE/DX =    0.0               !
! D71   D(11,12,13,14)         0.0            -DE/DX =    0.0               !
! D72   D(11,12,13,18)       177.1787         -DE/DX =    0.0               !
! D73   D(17,12,13,14)      -177.1787         -DE/DX =    0.0               !
! D74   D(17,12,13,18)         0.0            -DE/DX =    0.0               !
! D75   D(17,12,21,1)          40.9151         -DE/DX =    0.0               !
! D76   D(17,12,21,2)          0.0            -DE/DX =    0.0               !
! D77   D(17,12,21,3)        -40.9151         -DE/DX =    0.0               !
! D78   D(17,12,21,4)        -74.7635         -DE/DX =    0.0               !
! D79   D(17,12,21,5)         74.7635         -DE/DX =    0.0               !
! D80   D(17,12,21,14)      -158.8139         -DE/DX =    0.0               !
! D81   D(17,12,21,15)       158.8139         -DE/DX =    0.0               !
! D82   D(12,13,14,15)         0.0            -DE/DX =    0.0               !
! D83   D(12,13,14,19)       177.1787         -DE/DX =    0.0               !
! D84   D(18,13,14,15)      -177.1787         -DE/DX =    0.0               !
! D85   D(18,13,14,19)         0.0            -DE/DX =    0.0               !
! D86   D(18,13,21,1)          74.7635         -DE/DX =    0.0               !
! D87   D(18,13,21,2)          40.9151         -DE/DX =    0.0               !
! D88   D(18,13,21,3)          0.0            -DE/DX =    0.0               !
! D89   D(18,13,21,4)        -40.9151         -DE/DX =    0.0               !
! D90   D(18,13,21,5)        -74.7635         -DE/DX =    0.0               !
! D91   D(18,13,21,11)       158.8139         -DE/DX =    0.0               !
! D92   D(18,13,21,15)      -158.8139         -DE/DX =    0.0               !
! D93   D(13,14,15,11)         0.0            -DE/DX =    0.0               !
! D94   D(13,14,15,20)       177.1787         -DE/DX =    0.0               !
! D95   D(19,14,15,11)      -177.1787         -DE/DX =    0.0               !
! D96   D(19,14,15,20)         0.0            -DE/DX =    0.0               !
! D97   D(19,14,21,1)        -74.7635         -DE/DX =    0.0               !
! D98   D(19,14,21,2)         74.7635         -DE/DX =    0.0               !
```

```
! D99   D(19,14,21,3)          40.9151         -DE/DX =    0.0                 !
! D100  D(19,14,21,4)           0.0            -DE/DX =    0.0                 !
! D101  D(19,14,21,5)         -40.9151         -DE/DX =    0.0                 !
! D102  D(19,14,21,11)       -158.8139         -DE/DX =    0.0                 !
! D103  D(19,14,21,12)        158.8139         -DE/DX =    0.0                 !
! D104  D(20,15,21,1)         -40.9151         -DE/DX =    0.0                 !
! D105  D(20,15,21,2)         -74.7635         -DE/DX =    0.0                 !
! D106  D(20,15,21,3)          74.7635         -DE/DX =    0.0                 !
! D107  D(20,15,21,4)          40.9151         -DE/DX =    0.0                 !
! D108  D(20,15,21,5)           0.0            -DE/DX =    0.0                 !
! D109  D(20,15,21,12)       -158.8139         -DE/DX =    0.0                 !
! D110  D(20,15,21,13)        158.8139         -DE/DX =    0.0                 !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Dipole is zero, so no output in dipole orientation.

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

Electric dipole moment (input orientation):
(Debye = 10**-18 statcoulomb cm , SI units = C m)
                 (au)           (Debye)         (10**-30 SI)
  Tot        0.000000D+00      0.000000D+00      0.000000D+00
  x          0.000000D+00      0.000000D+00      0.000000D+00
  y          0.000000D+00      0.000000D+00      0.000000D+00
  z          0.000000D+00      0.000000D+00      0.000000D+00

Dipole polarizability, Alpha (input orientation).
(esu units = cm**3 , SI units = C**2 m**2 J**-1)
Alpha(0;0):
              (au)            (10**-24 esu)      (10**-40 SI)
  iso        0.115050D+03      0.170487D+02      0.189693D+02
  aniso      0.415486D+02      0.615687D+01      0.685044D+01
  xx         0.101201D+03      0.149964D+02      0.166857D+02
  yx         0.000000D+00      0.000000D+00      0.000000D+00
  yy         0.101201D+03      0.149965D+02      0.166858D+02
  zx         0.000000D+00      0.000000D+00      0.000000D+00
  zy         0.000000D+00      0.000000D+00      0.000000D+00
  zz         0.142749D+03      0.211533D+02      0.235362D+02

----------------------------------------------------------------------
1\1\GINC-COMET-08-37\Freq\RB3LYP\3-21G*\C10H10Ru1\GRIDCHEM\31-Jan-2021
\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/3-21G* Freq
\\<Calculation as sent>\\0,1\C,0.,1.22497398,-1.88346255\C,-1.16501948
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 ERROR IS A HARDY PLANT... IT FLOURISHETH IN EVERY SOIL.
            MARTIN FARQUHAR TUPPER
 Job cpu time:       0 days  0 hours 17 minutes 55.3 seconds.
 Elapsed time:       0 days  0 hours  1 minutes 19.8 seconds.
 File lengths (MBytes):  RWF=     82 Int=      0 D2E=      0 Chk=      4 Scr=
1
 Normal termination of Gaussian 16 at Sun Jan 31 22:52:02 2021.
```