```
 Entering Gaussian System, Link 0=/opt/software/gaussian/g16.a03/g16
 Initial command:
 /opt/software/gaussian/g16.a03/l1.exe "/scratch/jcanal/60199841/Gau-193859.inp"
-scrdir="/scratch/jcanal/60199841/"
 Entering Link 1 = /opt/software/gaussian/g16.a03/l1.exe PID=    193863.

 Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2009,2016,
            Gaussian, Inc.  All Rights Reserved.

 This is part of the Gaussian(R) 16 program.  It is based on
 the Gaussian(R) 09 system (copyright 2009, Gaussian, Inc.),
 the Gaussian(R) 03 system (copyright 2003, Gaussian, Inc.),
 the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),
 the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),
 the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),
 the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),
 the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),
 the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon
 University), and the Gaussian 82(TM) system (copyright 1983,
 Carnegie Mellon University). Gaussian is a federally registered
 trademark of Gaussian, Inc.

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

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

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

                      RESTRICTED RIGHTS LEGEND

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

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


 -------------------------------------------------------------
 Warning -- This program may not be used in any manner that
 competes with the business of Gaussian, Inc. or will provide
 assistance to any competitor of Gaussian, Inc.  The licensee
 of this program is prohibited from giving any competitor of
 Gaussian, Inc. access to this program.  By using this program,
 the user acknowledges that Gaussian, Inc. is engaged in the
```

business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.

Cite this work as:
Gaussian 16, Revision A.03,
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-G16RevA.03 25-Dec-2016
               21-Jan-2021
****
%chk=RuC5H5_8.chk
%mem=8000MB
%nproc=12
Will use up to   12 processors via shared memory.
----
nmr=giao b3lyp/3-21g* scrf=(solvent=chloroform) geom=connectivity
----
1/38=1,57=2,172=1/1;
2/12=2,17=6,18=5,40=1/2;
3/5=5,7=1,11=2,25=1,30=1,70=2201,72=7,74=-5/1,2,3,8;
4//1;
5/5=2,38=5,53=7/2;
8/6=1,10=90,11=11/1;
10/13=100,45=16/2;
6/7=2,8=2,9=2,10=2,28=1/1;
99/9=1/99;

<Calculation as sent>

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	0.00678	-1.22485	-1.88318
C	1.16699	-0.37205	-1.88318
C	0.71446	0.99491	-1.88318
C	-0.72543	0.98694	-1.88318
C	-1.1628	-0.38495	-1.88318
H	2.19373	-0.69921	-1.92636
H	1.34288	1.87029	-1.92636
H	-1.36378	1.85511	-1.92636
H	-2.18574	-0.72377	-1.92636
H	0.01291	-2.30242	-1.92636
C	-0.00678	-1.22485	1.88318
C	1.1628	-0.38495	1.88318
C	0.72543	0.98694	1.88318
C	-0.71446	0.99491	1.88318
C	-1.16699	-0.37205	1.88318
H	-0.01291	-2.30242	1.92636
H	2.18574	-0.72377	1.92636
H	1.36378	1.85511	1.92636
H	-1.34288	1.87029	1.92636
H	-2.19373	-0.69921	1.92636
Ru	0.	0.	0.

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.006778	-1.224847	-1.883181
2	6	0	1.166994	-0.372052	-1.883181
3	6	0	0.714463	0.994907	-1.883181
4	6	0	-0.725431	0.986938	-1.883181
5	6	0	-1.162804	-0.384945	-1.883181
6	1	0	2.193725	-0.699207	-1.926359
7	1	0	1.342884	1.870290	-1.926359
8	1	0	-1.363778	1.855110	-1.926359
9	1	0	-2.185745	-0.723769	-1.926359
10	1	0	0.012913	-2.302424	-1.926359
11	6	0	-0.006778	-1.224847	1.883181
12	6	0	1.162804	-0.384945	1.883181
13	6	0	0.725431	0.986938	1.883181
14	6	0	-0.714463	0.994907	1.883181
15	6	0	-1.166994	-0.372052	1.883181
16	1	0	-0.012913	-2.302424	1.926359
17	1	0	2.185745	-0.723769	1.926359
18	1	0	1.363778	1.855110	1.926359
19	1	0	-1.342884	1.870290	1.926359
20	1	0	-2.193725	-0.699207	1.926359
21	44	0	0.000000	0.000000	0.000000

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.439917	0.000000			
3	C	2.329834	1.439916	0.000000		
4	C	2.329834	2.329834	1.439916	0.000000	
5	C	1.439916	2.329834	2.329834	1.439916	0.000000
6	H	2.249644	1.078458	2.249467	3.371413	3.371486
7	H	3.371486	2.249644	1.078458	2.249467	3.371413
8	H	3.371413	3.371486	2.249644	1.078458	2.249467
9	H	2.249467	3.371413	3.371486	2.249644	1.078458
10	H	1.078458	2.249467	3.371413	3.371486	2.249644
11	C	3.766387	4.036147	4.430912	4.426504	4.028314
12	C	4.028314	3.766387	4.036147	4.430912	4.426504
13	C	4.426504	4.028314	3.766387	4.036147	4.430912
14	C	4.430912	4.426504	4.028314	3.766387	4.036147
15	C	4.036147	4.430912	4.426504	4.028314	3.766387
16	H	3.959060	4.430701	5.090585	5.083323	4.417190
17	H	4.417190	3.959060	4.430701	5.090585	5.083323
18	H	5.083323	4.417190	3.959060	4.430701	5.090585
19	H	5.090585	5.083323	4.417190	3.959060	4.430701
20	H	4.430701	5.090585	5.083323	4.417190	3.959060
21	Ru	2.246479	2.246479	2.246479	2.246479	2.246479

		6	7	8	9	10
6	H	0.000000				
7	H	2.706704	0.000000			
8	H	4.379539	2.706704	0.000000		
9	H	4.379539	4.379539	2.706704	0.000000	
10	H	2.706704	4.379539	4.379539	2.706704	0.000000
11	C	4.430701	5.090585	5.083323	4.417190	3.959060
12	C	3.959060	4.430701	5.090585	5.083323	4.417190
13	C	4.417190	3.959060	4.430701	5.090585	5.083323
14	C	5.083323	4.417190	3.959060	4.430701	5.090585
15	C	5.090585	5.083323	4.417190	3.959060	4.430701
16	H	4.720486	5.838935	5.826950	4.696465	3.852804
17	H	3.852804	4.720486	5.838935	5.826950	4.696465
18	H	4.696465	3.852804	4.720486	5.838935	5.826950
19	H	5.826950	4.696465	3.852804	4.720486	5.838935
20	H	5.838935	5.826950	4.696465	3.852804	4.720486
21	Ru	3.002029	3.002029	3.002029	3.002029	3.002029

		11	12	13	14	15
11	C	0.000000				
12	C	1.439916	0.000000			
13	C	2.329834	1.439916	0.000000		
14	C	2.329834	2.329834	1.439916	0.000000	
15	C	1.439917	2.329834	2.329834	1.439916	0.000000
16	H	1.078458	2.249644	3.371486	3.371413	2.249467
17	H	2.249467	1.078458	2.249644	3.371486	3.371413
18	H	3.371413	2.249467	1.078458	2.249644	3.371486
19	H	3.371486	3.371413	2.249467	1.078458	2.249644

```
   20  H    2.249644   3.371486   3.371413   2.249467   1.078458
   21  Ru   2.246479   2.246479   2.246479   2.246479   2.246479
                 16         17         18         19         20
   16  H    0.000000
   17  H    2.706704   0.000000
   18  H    4.379539   2.706704   0.000000
   19  H    4.379539   4.379539   2.706704   0.000000
   20  H    2.706704   4.379539   4.379539   2.706704   0.000000
   21  Ru   3.002029   3.002029   3.002029   3.002029   3.002029
                 21
   21  Ru   0.000000
 Stoichiometry    C10H10Ru
 Framework group  D5[O(Ru),X(C10H10)]
 Deg. of freedom     6
 Full point group                 D5      NOp  10
 Largest Abelian subgroup         C2      NOp   2
 Largest concise Abelian subgroup C2      NOp   2
                       Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        0.006778    1.224847    1.883181
      2          6           0        1.166994    0.372052    1.883181
      3          6           0        0.714463   -0.994907    1.883181
      4          6           0       -0.725431   -0.986938    1.883181
      5          6           0       -1.162804    0.384945    1.883181
      6          1           0        2.193725    0.699207    1.926359
      7          1           0        1.342884   -1.870290    1.926359
      8          1           0       -1.363778   -1.855110    1.926359
      9          1           0       -2.185745    0.723769    1.926359
     10          1           0        0.012913    2.302424    1.926359
     11          6           0       -0.006778    1.224847   -1.883181
     12          6           0        1.162804    0.384945   -1.883181
     13          6           0        0.725431   -0.986938   -1.883181
     14          6           0       -0.714463   -0.994907   -1.883181
     15          6           0       -1.166994    0.372052   -1.883181
     16          1           0       -0.012913    2.302424   -1.926359
     17          1           0        2.185745    0.723769   -1.926359
     18          1           0        1.363778   -1.855110   -1.926359
     19          1           0       -1.342884   -1.870290   -1.926359
     20          1           0       -2.193725    0.699207   -1.926359
     21         44           0        0.000000    0.000000    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.1647007           0.8718010
0.8718010
 Standard basis: 3-21G* (6D, 7F)
 There are    78 symmetry adapted cartesian basis functions of A   symmetry.
 There are    71 symmetry adapted cartesian basis functions of B   symmetry.
 There are    78 symmetry adapted basis functions of A   symmetry.
```

```
 There are    71 symmetry adapted basis functions of B   symmetry.
   149 basis functions,   267 primitive gaussians,   149 cartesian basis functions
    57 alpha electrons       57 beta electrons
       nuclear repulsion energy      1146.2969238525 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.
 ------------------------------------------------------------------------------
 Polarizable Continuum Model (PCM)
 =================================
 Model                : PCM.
 Atomic radii         : UFF (Universal Force Field).
 Polarization charges : Total charges.
 Charge compensation  : None.
 Solution method      : On-the-fly selection.
 Cavity type          : Scaled VdW (van der Waals Surface) (Alpha=1.100).
 Cavity algorithm     : GePol (No added spheres)
                        Default sphere list used, NSphG=   21.
                        Lebedev-Laikov grids with approx.  5.0 points / Ang**2.
                        Smoothing algorithm: York/Karplus (Gamma=1.0000).
                        Polarization charges: spherical gaussians, with
                                              point-specific exponents (IZeta= 3).
                        Self-potential: point-specific (ISelfS= 7).
                        Self-field    : sphere-specific E.n sum rule (ISelfD= 2).
 Solvent              : Chloroform, Eps=   4.711300 Eps(inf)=   2.090627
 ------------------------------------------------------------------------------
 One-electron integrals computed using PRISM.
 NBasis=   149 RedAO= T EigKep=  1.33D-03  NBF=    78    71
 NBsUse=   149 1.00D-06 EigRej= -1.00D+00 NBFU=    78    71
 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.
 Initial guess orbital symmetries:
       Occupied  (A1) (A1) (A2) (E1) (E1) (A1) (A2) (E1) (E1) (E2)
                 (E2) (E2) (E2) (E1) (E1) (A2) (E1) (E1) (A1) (E1)
                 (E1) (A1) (E2) (E2) (A1) (A2) (E1) (E1) (A1) (A2)
                 (E1) (E1) (E1) (E1) (E2) (E2) (E2) (E2) (A1) (A2)
```

```
                (E1) (E1) (E1) (E1) (E2) (E2) (E2) (E2) (A1) (A2)
                (E1) (E1) (E1) (E1) (E2) (E2) (A1)
      Virtual   (E2) (E2) (E1) (E1) (E2) (E2) (A1) (E1) (E1) (A2)
                (E1) (E1) (E2) (E2) (E2) (E2) (A2) (E1) (E1) (A1)
                (E1) (E1) (E1) (E1) (A1) (E1) (E1) (E2) (E2) (E2)
                (E2) (A2) (A1) (A1) (A2) (E2) (E2) (E2) (E2) (E1)
                (E1) (A2) (E1) (E1) (A1) (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) (E2) (E2) (E2) (E2) (E1) (E1) (A1)
                (A1) (E1) (E1) (E2) (E2) (A2) (E1) (E1) (E2) (E2)
                (A1) (A1)
The electronic state of the initial guess is 1-A1.
Keep R1 ints in memory in symmetry-blocked form, NReq=93700165.
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.
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.
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.
Defaulting to unpruned grid for atomic number  44.
Inv3:  Mode=1 IEnd=     8885523.
Iteration    1 A*A^-1 deviation from unit magnitude is 3.22D-15 for   1136.
Iteration    1 A*A^-1 deviation from orthogonality  is 2.05D-15 for   1303    343.
Iteration    1 A^-1*A deviation from unit magnitude is 3.33D-15 for    561.
Iteration    1 A^-1*A deviation from orthogonality  is 1.99D-15 for   1293    369.
Density matrix breaks symmetry, PCut= 1.00D-04
Density has only Abelian symmetry.
Density matrix breaks symmetry, PCut= 1.00D-04
Density has only Abelian symmetry.
EnCoef did   100 forward-backward iterations
Density matrix breaks symmetry, PCut= 1.00D-04
Density has only Abelian symmetry.
Density matrix breaks symmetry, PCut= 1.00D-04
Density has only Abelian symmetry.
Density matrix breaks symmetry, PCut= 1.00D-04
Density has only Abelian symmetry.
Density matrix breaks symmetry, PCut= 1.00D-04
Density has only Abelian symmetry.
Density matrix breaks symmetry, PCut= 1.00D-04
Density has only Abelian symmetry.
```

```
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 Error on total polarization charges =  0.00529
 SCF Done:  E(RB3LYP) =  -4808.20995893     A.U. after   13 cycles
            NFock= 13  Conv=0.18D-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  0.20105576D+02

 NEqPCM:  Using equilibrium solvation (IEInf=0, Eps=   4.7113, EpsInf=   2.0906)
          Differentiating once with respect to magnetic field using GIAOs.
          Electric field/nuclear overlap derivatives assumed to be zero.
 Defaulting to unpruned grid for atomic number  44.
 Keep R3 ints in memory in symmetry-blocked form, NReq=93708520.
 FoFJK:  IHMeth= 1 ICntrl=    6127 DoSepK=F KAlg= 0 I1Cent=           0 FoldK=F
 IRaf=         1 NMat=       1 IRICut=       1 DoRegI=T DoRafI=F ISym2E= 0 IDoP0=0
IntGTp=1.
 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.
 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.
 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.
 Defaulting to unpruned grid for atomic number  44.
          There are     3 degrees of freedom in the 1st order CPHF.  IDoFFX=0
NUNeed=     3.
      3 vectors produced by pass  0 Test12= 1.75D-13 3.33D-08 XBig12= 2.09D+01
1.84D+00.
 AX will form     3 AO Fock derivatives at one time.
      3 vectors produced by pass  1 Test12= 1.75D-13 3.33D-08 XBig12= 3.07D-01
4.16D-01.
      3 vectors produced by pass  2 Test12= 1.75D-13 3.33D-08 XBig12= 2.70D-03
1.25D-02.
      3 vectors produced by pass  3 Test12= 1.75D-13 3.33D-08 XBig12= 2.05D-05
```

```
2.05D-03.
      3 vectors produced by pass  4 Test12= 1.75D-13 3.33D-08 XBig12= 4.69D-07
2.67D-04.
      3 vectors produced by pass  5 Test12= 1.75D-13 3.33D-08 XBig12= 1.48D-09
8.35D-06.
      2 vectors produced by pass  6 Test12= 1.75D-13 3.33D-08 XBig12= 3.05D-12
7.30D-07.
      2 vectors produced by pass  7 Test12= 1.75D-13 3.33D-08 XBig12= 8.09D-15
3.80D-08.
 InvSVY:  IOpt=1 It=  1 EMax= 8.88D-16
 Solved reduced A of dimension    22 with     3 vectors.
 Calculating GIAO nuclear magnetic shielding tensors.
 SCF GIAO Magnetic shielding tensor (ppm):
      1  C    Isotropic =   133.8935   Anisotropy =    76.7841
   XX=   129.0353   YX=    -0.2020   ZX=    -0.0081
   XY=    -0.2022   YY=    91.6177   ZY=    -2.6363
   XZ=    -0.2205   YZ=   -36.3007   ZZ=   181.0276
   Eigenvalues:    87.5613   129.0363   185.0829
      2  C    Isotropic =   133.8974   Anisotropy =    76.7673
   XX=    95.0837   YX=   -10.8310   ZX=    -2.5078
   XY=   -10.8370   YY=   125.5892   ZY=    -0.7999
   XZ=   -34.5979   YZ=   -11.0078   ZZ=   181.0192
   Eigenvalues:    87.5712   129.0453   185.0756
      3  C    Isotropic =   133.9057   Anisotropy =    76.7763
   XX=   116.3165   YX=    17.7265   ZX=    -1.5423
   XY=    17.7275   YY=   104.3743   ZY=     2.1714
   XZ=   -21.1757   YZ=    29.4968   ZZ=   181.0263
   Eigenvalues:    87.5761   129.0511   185.0899
      4  C    Isotropic =   133.9048   Anisotropy =    76.7827
   XX=   115.9305   YX=   -17.8542   ZX=     1.5699
   XY=   -17.8529   YY=   104.7559   ZY=     2.1639
   XZ=    21.5314   YZ=    29.2368   ZZ=   181.0282
   Eigenvalues:    87.5707   129.0506   185.0933
      5  C    Isotropic =   133.8967   Anisotropy =    76.7743
   XX=    95.3169   YX=    11.1588   ZX=     2.5151
   XY=    11.1660   YY=   125.3523   ZY=    -0.8214
   XZ=    34.4609   YZ=   -11.4256   ZZ=   181.0209
   Eigenvalues:    87.5642   129.0464   185.0795
      6  H    Isotropic =    28.8341   Anisotropy =    11.1424
   XX=    34.1754   YX=     3.1598   ZX=     3.8452
   XY=     3.1618   YY=    25.2747   ZY=     1.2257
   XZ=     2.1613   YZ=     0.6885   ZZ=    27.0523
   Eigenvalues:    24.2664    25.9735    36.2624
      7  H    Isotropic =    28.8339   Anisotropy =    11.1445
   XX=    27.9805   YX=    -5.1741   ZX=     2.3539
   XY=    -5.1743   YY=    31.4682   ZY=    -3.2789
   XZ=     1.3244   YZ=    -1.8421   ZZ=    27.0530
   Eigenvalues:    24.2642    25.9740    36.2636
      8  H    Isotropic =    28.8337   Anisotropy =    11.1441
   XX=    28.0915   YX=     5.2095   ZX=    -2.3906
```

```
XY=     5.2103   YY=    31.3567   ZY=    -3.2529
XZ=    -1.3451   YZ=    -1.8273   ZZ=    27.0530
Eigenvalues:    24.2644    25.9736    36.2632
   9  H    Isotropic =    28.8339   Anisotropy =    11.1420
XX=    34.1059   YX=    -3.2545   ZX=    -3.8320
XY=    -3.2560   YY=    25.3437   ZY=     1.2677
XZ=    -2.1538   YZ=     0.7126   ZZ=    27.0521
Eigenvalues:    24.2667    25.9731    36.2619
  10  H    Isotropic =    28.8342   Anisotropy =    11.1409
XX=    24.2673   YX=     0.0583   ZX=     0.0226
XY=     0.0588   YY=    35.1825   ZY=     4.0338
XZ=     0.0127   YZ=     2.2695   ZZ=    27.0529
Eigenvalues:    24.2670    25.9742    36.2615
  11  C    Isotropic =   133.8935   Anisotropy =    76.7841
XX=   129.0353   YX=     0.2020   ZX=    -0.0081
XY=     0.2022   YY=    91.6177   ZY=     2.6363
XZ=    -0.2205   YZ=    36.3007   ZZ=   181.0276
Eigenvalues:    87.5613   129.0363   185.0829
  12  C    Isotropic =   133.8967   Anisotropy =    76.7743
XX=    95.3169   YX=   -11.1588   ZX=     2.5151
XY=   -11.1660   YY=   125.3523   ZY=     0.8214
XZ=    34.4609   YZ=    11.4256   ZZ=   181.0209
Eigenvalues:    87.5642   129.0464   185.0795
  13  C    Isotropic =   133.9048   Anisotropy =    76.7827
XX=   115.9305   YX=    17.8542   ZX=     1.5699
XY=    17.8529   YY=   104.7559   ZY=    -2.1639
XZ=    21.5314   YZ=   -29.2368   ZZ=   181.0282
Eigenvalues:    87.5707   129.0506   185.0933
  14  C    Isotropic =   133.9057   Anisotropy =    76.7763
XX=   116.3165   YX=   -17.7265   ZX=    -1.5423
XY=   -17.7275   YY=   104.3743   ZY=    -2.1714
XZ=   -21.1757   YZ=   -29.4968   ZZ=   181.0263
Eigenvalues:    87.5761   129.0511   185.0899
  15  C    Isotropic =   133.8974   Anisotropy =    76.7673
XX=    95.0837   YX=    10.8310   ZX=    -2.5078
XY=    10.8370   YY=   125.5892   ZY=     0.7999
XZ=   -34.5979   YZ=    11.0078   ZZ=   181.0192
Eigenvalues:    87.5712   129.0453   185.0756
  16  H    Isotropic =    28.8342   Anisotropy =    11.1409
XX=    24.2673   YX=    -0.0583   ZX=     0.0226
XY=    -0.0588   YY=    35.1825   ZY=    -4.0338
XZ=     0.0127   YZ=    -2.2695   ZZ=    27.0529
Eigenvalues:    24.2670    25.9742    36.2615
  17  H    Isotropic =    28.8339   Anisotropy =    11.1420
XX=    34.1059   YX=     3.2545   ZX=    -3.8320
XY=     3.2560   YY=    25.3437   ZY=    -1.2677
XZ=    -2.1538   YZ=    -0.7126   ZZ=    27.0521
Eigenvalues:    24.2667    25.9731    36.2619
  18  H    Isotropic =    28.8337   Anisotropy =    11.1441
XX=    28.0915   YX=    -5.2095   ZX=    -2.3906
```

```
  XY=    -5.2103   YY=    31.3567   ZY=     3.2529
  XZ=    -1.3451   YZ=     1.8273   ZZ=    27.0530
  Eigenvalues:    24.2644    25.9736    36.2632
    19  H    Isotropic =    28.8339   Anisotropy =    11.1445
  XX=    27.9805   YX=     5.1741   ZX=     2.3539
  XY=     5.1743   YY=    31.4682   ZY=     3.2789
  XZ=     1.3244   YZ=     1.8421   ZZ=    27.0530
  Eigenvalues:    24.2642    25.9740    36.2636
    20  H    Isotropic =    28.8341   Anisotropy =    11.1424
  XX=    34.1754   YX=    -3.1598   ZX=     3.8452
  XY=    -3.1618   YY=    25.2747   ZY=    -1.2257
  XZ=     2.1613   YZ=    -0.6885   ZZ=    27.0523
  Eigenvalues:    24.2664    25.9735    36.2624
    21  Ru   Isotropic =     3.2760   Anisotropy =  5252.8864
  XX= -1746.3391   YX=     0.0000   ZX=    -0.0064
  XY=     0.0000   YY= -1749.0332   ZY=    -0.0000
  XZ=     0.0087   YZ=     0.0000   ZZ=  3505.2003
  Eigenvalues: -1749.0332 -1746.3391  3505.2003
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.
SCF density gives NOpUse=  2 NOpAll= 10.

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

           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) (?A) (?A) (?A) (?A)
                (?A) (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)
Unable to determine electronic state:  an orbital has unidentified symmetry.
Alpha  occ. eigenvalues -- -781.89556-111.31022-102.63522-102.62853-102.62853
Alpha  occ. eigenvalues --  -19.87936 -16.30714 -16.29207 -16.29206 -10.49611
Alpha  occ. eigenvalues --  -10.49384 -10.49384 -10.48399 -10.48399 -10.13978
```

```
Alpha  occ. eigenvalues --  -10.13977 -10.13947 -10.13947 -10.13943 -10.13941
Alpha  occ. eigenvalues --  -10.13941 -10.13918 -10.13918 -10.13856  -2.74923
Alpha  occ. eigenvalues --   -1.70261  -1.65194  -1.65193  -0.89452  -0.87752
Alpha  occ. eigenvalues --   -0.71924  -0.71924  -0.71276  -0.71275  -0.55031
Alpha  occ. eigenvalues --   -0.55031  -0.54590  -0.54590  -0.54068  -0.52940
Alpha  occ. eigenvalues --   -0.41911  -0.41911  -0.40764  -0.40764  -0.40629
Alpha  occ. eigenvalues --   -0.38527  -0.38526  -0.38313  -0.38313  -0.36051
Alpha  occ. eigenvalues --   -0.29198  -0.29198  -0.23579  -0.23579  -0.21590
Alpha  occ. eigenvalues --   -0.19994  -0.19994
Alpha virt. eigenvalues --   -0.00733  -0.00733   0.02573   0.03572   0.03574
Alpha virt. eigenvalues --    0.05096   0.05476   0.05477   0.08235   0.08236
Alpha virt. eigenvalues --    0.16522   0.17004   0.18617   0.18618   0.19390
Alpha virt. eigenvalues --    0.19390   0.19588   0.19588   0.19931   0.19935
Alpha virt. eigenvalues --    0.24171   0.24173   0.24841   0.24841   0.25553
Alpha virt. eigenvalues --    0.30880   0.30881   0.38720   0.38720   0.39330
Alpha virt. eigenvalues --    0.39330   0.43935   0.44209   0.44278   0.49685
Alpha virt. eigenvalues --    0.69255   0.69256   0.71191   0.71191   0.71341
Alpha virt. eigenvalues --    0.71342   0.76216   0.76611   0.77396   0.77396
Alpha virt. eigenvalues --    0.79207   0.79208   0.83374   0.83375   0.86029
Alpha virt. eigenvalues --    0.87651   0.87652   0.90921   0.96260   0.96260
Alpha virt. eigenvalues --    0.98007   0.98007   0.98591   0.98592   1.00668
Alpha virt. eigenvalues --    1.01706   1.05298   1.05298   1.10200   1.10201
Alpha virt. eigenvalues --    1.17514   1.19559   1.19634   1.19634   1.25739
Alpha virt. eigenvalues --    1.25739   1.34307   1.34308   1.36172   1.37213
Alpha virt. eigenvalues --    1.37214   1.38431   1.38432   1.39267   1.39268
Alpha virt. eigenvalues --    1.93080   1.99995   1.99997   2.01903   2.01903
Alpha virt. eigenvalues --    2.28443   2.42116   2.42116   2.43219   2.43219
Alpha virt. eigenvalues --    3.23816 152.26681
         Condensed to atoms (all electrons):
              1          2          3          4          5          6
    1  C    5.489771   0.356934  -0.119804  -0.119804   0.356935  -0.027911
    2  C    0.356934   5.489800   0.356922  -0.119795  -0.119806   0.398747
    3  C   -0.119804   0.356922   5.489853   0.356868  -0.119795  -0.027938
    4  C   -0.119804  -0.119795   0.356868   5.489852   0.356924   0.003066
    5  C    0.356935  -0.119806  -0.119795   0.356924   5.489796   0.003064
    6  H   -0.027911   0.398747  -0.027938   0.003066   0.003064   0.447445
    7  H    0.003064  -0.027909   0.398746  -0.027941   0.003066  -0.001474
    8  H    0.003066   0.003064  -0.027915   0.398746  -0.027934  -0.000016
    9  H   -0.027936   0.003066   0.003064  -0.027913   0.398747  -0.000016
   10  H    0.398747  -0.027939   0.003067   0.003064  -0.027913  -0.001474
   11  C    0.008140  -0.001818  -0.000641  -0.000668  -0.001746  -0.000034
   12  C   -0.001746   0.008140  -0.001818  -0.000641  -0.000668  -0.000276
   13  C   -0.000668  -0.001745   0.008138  -0.001820  -0.000641  -0.000037
   14  C   -0.000641  -0.000668  -0.001748   0.008138  -0.001818  -0.000000
   15  C   -0.001818  -0.000641  -0.000668  -0.001745   0.008140  -0.000000
   16  H   -0.000276  -0.000034  -0.000000  -0.000000  -0.000037   0.000001
   17  H   -0.000037  -0.000276  -0.000034  -0.000000  -0.000000   0.000006
   18  H   -0.000000  -0.000037  -0.000276  -0.000034  -0.000000   0.000001
   19  H   -0.000000  -0.000000  -0.000037  -0.000276  -0.000034   0.000000
   20  H   -0.000034  -0.000000  -0.000000  -0.000037  -0.000276   0.000000
```

21	Ru	-0.012439	-0.012448	-0.012408	-0.012410	-0.012449	-0.005544
		7	8	9	10	11	12
1	C	0.003064	0.003066	-0.027936	0.398747	0.008140	-0.001746
2	C	-0.027909	0.003064	0.003066	-0.027939	-0.001818	0.008140
3	C	0.398746	-0.027915	0.003064	0.003067	-0.000641	-0.001818
4	C	-0.027941	0.398746	-0.027913	0.003064	-0.000668	-0.000641
5	C	0.003066	-0.027934	0.398747	-0.027913	-0.001746	-0.000668
6	H	-0.001474	-0.000016	-0.000016	-0.001474	-0.000034	-0.000276
7	H	0.447436	-0.001474	-0.000016	-0.000016	-0.000000	-0.000034
8	H	-0.001474	0.447435	-0.001474	-0.000016	-0.000000	-0.000000
9	H	-0.000016	-0.001474	0.447443	-0.001474	-0.000037	-0.000000
10	H	-0.000016	-0.000016	-0.001474	0.447436	-0.000276	-0.000037
11	C	-0.000000	-0.000000	-0.000037	-0.000276	5.489771	0.356935
12	C	-0.000034	-0.000000	-0.000000	-0.000037	0.356935	5.489796
13	C	-0.000276	-0.000034	-0.000000	-0.000000	-0.119804	0.356924
14	C	-0.000037	-0.000276	-0.000034	-0.000000	-0.119804	-0.119795
15	C	-0.000000	-0.000037	-0.000276	-0.000034	0.356934	-0.119806
16	H	0.000000	0.000000	0.000001	0.000006	0.398747	-0.027913
17	H	0.000001	0.000000	0.000000	0.000001	-0.027936	0.398747
18	H	0.000006	0.000001	0.000000	0.000000	0.003066	-0.027934
19	H	0.000001	0.000006	0.000001	0.000000	0.003064	0.003066
20	H	0.000000	0.000001	0.000006	0.000001	-0.027911	0.003064
21	Ru	-0.005548	-0.005548	-0.005544	-0.005542	-0.012439	-0.012449
		13	14	15	16	17	18
1	C	-0.000668	-0.000641	-0.001818	-0.000276	-0.000037	-0.000000
2	C	-0.001745	-0.000668	-0.000641	-0.000034	-0.000276	-0.000037
3	C	0.008138	-0.001748	-0.000668	-0.000000	-0.000034	-0.000276
4	C	-0.001820	0.008138	-0.001745	-0.000000	-0.000000	-0.000034
5	C	-0.000641	-0.001818	0.008140	-0.000037	-0.000000	-0.000000
6	H	-0.000037	-0.000000	-0.000000	0.000001	0.000006	0.000001
7	H	-0.000276	-0.000037	-0.000000	0.000000	0.000001	0.000006
8	H	-0.000034	-0.000276	-0.000037	0.000000	0.000000	0.000001
9	H	-0.000000	-0.000034	-0.000276	0.000001	0.000000	0.000000
10	H	-0.000000	-0.000000	-0.000034	0.000006	0.000001	0.000000
11	C	-0.119804	-0.119804	0.356934	0.398747	-0.027936	0.003066
12	C	0.356924	-0.119795	-0.119806	-0.027913	0.398747	-0.027934
13	C	5.489852	0.356868	-0.119795	0.003064	-0.027913	0.398746
14	C	0.356868	5.489853	0.356922	0.003067	0.003064	-0.027915
15	C	-0.119795	0.356922	5.489800	-0.027939	0.003066	0.003064
16	H	0.003064	0.003067	-0.027939	0.447436	-0.001474	-0.000016
17	H	-0.027913	0.003064	0.003066	-0.001474	0.447443	-0.001474
18	H	0.398746	-0.027915	0.003064	-0.000016	-0.001474	0.447435
19	H	-0.027941	0.398746	-0.027909	-0.000016	-0.000016	-0.001474
20	H	0.003066	-0.027938	0.398747	-0.001474	-0.000016	-0.000016
21	Ru	-0.012410	-0.012408	-0.012448	-0.005542	-0.005544	-0.005548
		19	20	21			
1	C	-0.000000	-0.000034	-0.012439			
2	C	-0.000000	-0.000000	-0.012448			
3	C	-0.000037	-0.000000	-0.012408			
4	C	-0.000276	-0.000037	-0.012410			

```
     5  C   -0.000034  -0.000276  -0.012449
     6  H    0.000000   0.000000  -0.005544
     7  H    0.000001   0.000000  -0.005548
     8  H    0.000006   0.000001  -0.005548
     9  H    0.000001   0.000006  -0.005544
    10  H    0.000000   0.000001  -0.005542
    11  C    0.003064  -0.027911  -0.012439
    12  C    0.003066   0.003064  -0.012449
    13  C   -0.027941   0.003066  -0.012410
    14  C    0.398746  -0.027938  -0.012408
    15  C   -0.027909   0.398747  -0.012448
    16  H   -0.000016  -0.001474  -0.005542
    17  H   -0.000016  -0.000016  -0.005544
    18  H   -0.001474  -0.000016  -0.005548
    19  H    0.447436  -0.001474  -0.005548
    20  H   -0.001474   0.447445  -0.005544
    21  Ru  -0.005548  -0.005544  43.268137
Mulliken charges:
             1
     1  C   -0.303542
     2  C   -0.303556
     3  C   -0.303575
     4  C   -0.303574
     5  C   -0.303555
     6  H    0.212391
     7  H    0.212405
     8  H    0.212406
     9  H    0.212392
    10  H    0.212400
    11  C   -0.303542
    12  C   -0.303555
    13  C   -0.303574
    14  C   -0.303575
    15  C   -0.303556
    16  H    0.212400
    17  H    0.212392
    18  H    0.212406
    19  H    0.212405
    20  H    0.212391
    21  Ru   0.911620
Sum of Mulliken charges =  -0.00000
Mulliken charges with hydrogens summed into heavy atoms:
             1
     1  C   -0.091142
     2  C   -0.091165
     3  C   -0.091171
     4  C   -0.091169
     5  C   -0.091163
    11  C   -0.091142
    12  C   -0.091163
```

```
    13  C   -0.091169
    14  C   -0.091171
    15  C   -0.091165
    21  Ru   0.911620
 Electronic spatial extent (au):  <R**2>=           1579.1425
 Charge=             -0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=              0.0000    Y=              0.0022    Z=              0.0000
Tot=              0.0022
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=            -74.4034   YY=            -74.4045   ZZ=            -87.9086
   XY=              0.0000   XZ=             -0.0001   YZ=              0.0000
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=              4.5021   YY=              4.5010   ZZ=             -9.0031
   XY=              0.0000   XZ=             -0.0001   YZ=              0.0000
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=              0.0000  YYY=              0.0072  ZZZ=             -0.0000
XYY=             -0.0000
  XXY=              0.0012  XXZ=              0.0000  XZZ=              0.0000
YZZ=              0.0015
  YYZ=              0.0000  XYZ=             -0.0000
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=           -379.4291 YYYY=           -379.4333 ZZZZ=          -1525.1048
XXXY=              0.0000
 XXXZ=             -0.0004 YYYX=              0.0000 YYYZ=             -0.0000
ZZZX=             -0.0005
 ZZZY=              0.0000 XXYY=           -126.4766 XXZZ=           -272.3665
YYZZ=           -272.3655
 XXYZ=              0.0000 YYXZ=             -0.0002 ZZXY=              0.0000
 N-N= 1.146296923853D+03 E-N=-1.369735661849D+04  KE= 4.784564157944D+03
 Symmetry A    KE= 3.368073896470D+03
 Symmetry B    KE= 1.416490261474D+03
 1\1\GINC-CDR1616\SP\RB3LYP\3-21G*\C10H10Ru1\JCANAL\21-Jan-2021\0\\# nm
 r=giao b3lyp/3-21g* scrf=(solvent=chloroform) geom=connectivity\\<Calc
 ulation as sent>\\0,1\C,0,0.00677848,-1.22484738,-1.88318113\C,0,1.166
 99375,-0.37205194,-1.88318113\C,0,0.71446332,0.99490663,-1.88318113\C,
 0,-0.72543113,0.98693805,-1.88318113\C,0,-1.16280441,-0.38494537,-1.88
 318113\H,0,2.19372534,-0.69920702,-1.92635881\H,0,1.3428838,1.87028993
 ,-1.92635881\H,0,-1.3637775,1.85510976,-1.92635881\H,0,-2.18574465,-0.
 72376904,-1.92635881\H,0,0.01291302,-2.30242363,-1.92635881\C,0,-0.006
 77848,-1.22484738,1.88318113\C,0,1.16280441,-0.38494537,1.88318113\C,0
 ,0.72543113,0.98693805,1.88318113\C,0,-0.71446332,0.99490663,1.8831811
 3\C,0,-1.16699375,-0.37205194,1.88318113\H,0,-0.01291302,-2.30242363,1
 .92635881\H,0,2.18574465,-0.72376904,1.92635881\H,0,1.3637775,1.855109
 76,1.92635881\H,0,-1.3428838,1.87028993,1.92635881\H,0,-2.19372534,-0.
 69920702,1.92635881\Ru,0,0.,0.,0.\\Version=ES64L-G16RevA.03\State=1-A1
 \HF=-4808.2099589\RMSD=1.757e-09\Dipole=0.,-0.0008793,0.\Quadrupole=3.
 3471972,3.3463585,-6.6935557,0.,0.0000856,0.\PG=D05 [O(Ru1),X(C10H10)]
 \\@
```

ALMOST ANYTHING IS EASIER TO GET INTO THAN OUT OF.

-- AGNES ALLEN'S LAW FROM
PAUL DICKSON'S "THE OFFICIAL RULES"

Job cpu time: 0 days 1 hours 24 minutes 46.0 seconds.
Elapsed time: 0 days 0 hours 7 minutes 47.7 seconds.
File lengths (MBytes): RWF= 62 Int= 0 D2E= 0 Chk= 4 Scr=
1
Normal termination of Gaussian 16 at Thu Jan 21 13:30:50 2021.