SUPPORTING INFORMATION

Spin dependent electrochemistry: focus on chiral vs achiral charge transmission through 2D SAMs adsorbed on gold.

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1. D-cysteine CVs and LSV

Figure 1SI shows cyclic voltammetry curves of D-cysteine as a function of the potential scan rate. They are reported to allow a close comparison with the L-cysteine electrochemical behaviour, please compare Figure 1 of the main manuscript

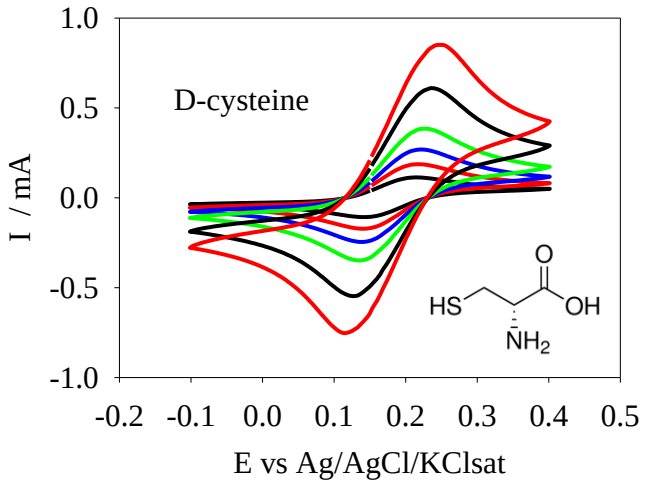

Figure 1SI.CV curves Fe3Fe2 5 mM solution, 0.5 M KCl in water as a function of the scan rate: 10, 25, 50, 100, 250, 500 mV/S. Working electrode gold functionalized with D-cysteine. Inset shows the D-cysteine molecular structure.

Figure 2SI shows a linear potential scan (LSV) curve of D-cysteine SAM adsorbed on gold, a clear electrodesorption peak is evident at $-0.71\ V$. Integration of the LSV curve allows to estimate the area

of a single molecule (based on the assumption that the electrodesorption of one molecule is equivalent, one-to-one, to the charge of $1.6 \times 10^{-19}\ C$). In the case of the electrodesorption of D-cysteine, shown in Figure 2SI, the surface area of a single molecule adsorbed on gold results of about $0.21\ nm^2 \pm 2$, a value in agreement with a good-quality monolayer of D-cysteine (as can be obtained by projecting the D-cysteine Van der Waals molecular model).

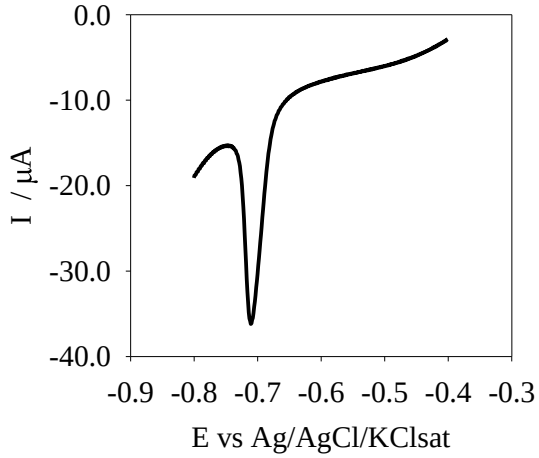

Figure 2SI. Linear scan potential (LSV) curve, 0.5 M KCl in water, 20 mV/S. Working electrode gold functionalized with D-cysteine. Surface WE area of 11 mm^2.

2. X-ray photo-electron spectroscopy (XPS) measurements

X-ray photo electron spectroscopy measurements were carried out at normal emission, with a VG XR3 double anode, and a X ray source delivering Mg Ka photons at 15 kV when operated with a 15 mA current. A CLAM2 VG hemispherical analyser driven at constant pass energy of 30 eV was employed. Survey spectra were recorded with an analyser resolution of 2 eV. Sulphur elemental spectra feature a higher resolution of 0.5 eV.

Figure 3SI sets out XPS spectra for gold surfaces functionalized with D- and L- cysteine. The relevant spectra show, for both compounds, typical S2p related features. These have been decomposed through fitting in spin-orbit split components, considering a spin orbit splitting between 2p1/2 and 2p3/2 of 1.2 eV and a branching ratio of 0.5. In the D-cysteine sample the S2 component is dominant. This result has to be ascribed to the formation of a single layer of molecules. This layer appears to be thinner with respect to the L-cysteine case, presumably due to differences in the effectiveness of the rinsing procedure. The L-cysteine sample, in fact, presents more intense S3 features from likely unbound thiol groups. This indicates that the effective thickness slightly exceeds the single layer. This is also consistent with the slightly higher intensity of the Au 4f peaks from the substrate, which are less damped by the organic film [1,2].

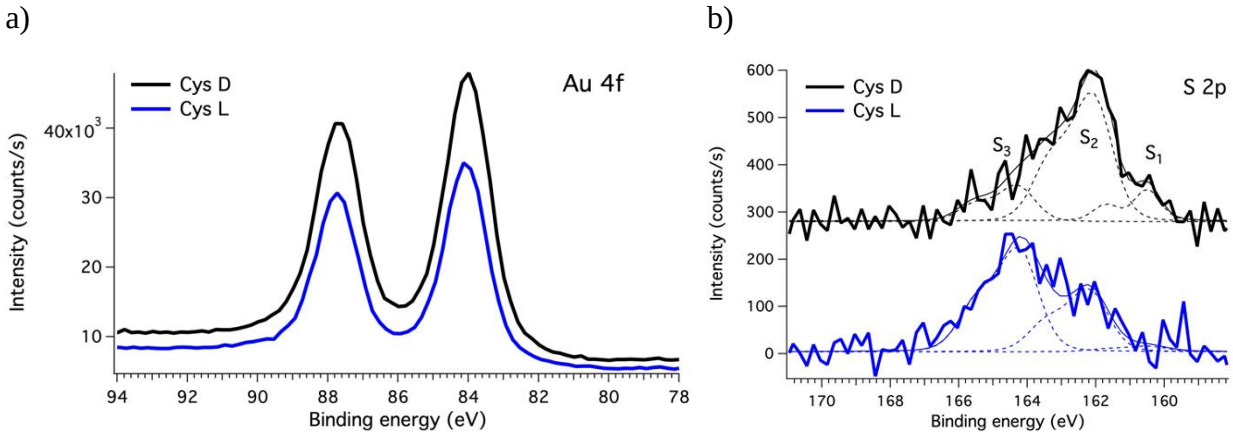

Figure 3SI. XPS elemental spectra of a) gold b) sulphur

3. Potassium hexacyanoferrate(II)/potassium hexacyanoferrate(III) redox couple spin state.

The chemistry of iron is all but a trivial subject, this is due to its complex electronic configuration [3,4]. The iron electronic configuration in the case of the Fe(II) species is an even electrons one: $3d^6 4s^0$, considering only the valence electrons. Trivial electron pairing following Hund's rule of the six iron valence electrons in the $3d$ atomic orbitals, should lead to a high-spin quartet. Indeed, the strong chemical interaction, in the hexacyanoferrate(II) anion $[Fe(CN)_6]^{4-}$, between the cyanide and Fe(II) leads to a closed-shell electronic configuration. Where, the $[Fe(CN)_6]^{4-}$ anion complex is characterized by an octahedral geometry, which features a A_{1g} low-spin singlet ground state $\ldots\left(\sigma(e_g)\right)^4\left(3d(t_{2g})\right)^6\left(\sigma^*(e_g)\right)^0\left(\pi^*_{CN}(t_{2g})\right)^0\ldots$ [5]. With evidence of a prominent ligand-to-metal and metal-to-ligand charge-transfer (σ-donation and π-back-donation) [6]. Furthermore, the iron electronic configuration in the case of the Fe(III) species is $3d^5 4s^0$, considering only the valence electrons. Again, the straightforward application of Hund's rule to the five valence electrons in the $3d$ atomic orbitals, should lead to a high-spin quintet. But even in this case the strong cyanide-iron chemical interaction yields a low-spin doublet as the final more stable electronic configuration for the ground state: $\ldots\left(\sigma(e_g)\right)^4\left(3d(t_{2g})\right)^5\left(\sigma^*(e_g)\right)^0\left(\pi^*_{CN}(t_{2g})\right)^0\ldots$. A detailed experimental (resonant inelastic X-ray scattering measurements) compared with theoretical ab-initio restricted active space multiconfigurational molecular orbital method, RAS [7].

4. On the relationship between optical rotation (OR), molecular properties (quantum mechanical based calculation of OR) and chirality.

The search of a quantitative method to weight the chirality of a compound is not at all a trivial matter [8]. In a totally empirical and arbitrary way, a reasonable yardstick to assess the manifestation of chirality is based on the measurement and comparison of optical rotation (OR) values. Optical rotation values are usually reported as the specific optical rotation (specific optical rotatory power): $[\alpha] = \alpha V/ml$, where α is the rotation of the polarization plane with respect to the original orientation, l is the length of the optical path, m is the mass of the sample, V is the volume. The connection to the molecular electronic structure goes through relationship: $[\alpha] = 288 \times 10^{-30}\pi^2 N_A a_0^4 \omega^2 \beta/M$, where N_A is the Avogadro's number, a_0 is the Bohr radius, M is the molecular molar mass, ω is the frequency of the light in atomic units, $\beta$is the trace of the Rosenberg tensor $\beta = (1/3)\mathrm{Tr}\beta_{\alpha\beta}$ [9]. The Rosenfeld tensor is related to the electric dipole – magnetic dipole polarizability $G_{\alpha\beta}$, $\beta_{\alpha\beta}(\omega) = -\omega^{-1}G_{\alpha\beta}(\omega)$. The electric dipole – magnetic dipole polarizability is the key quantity for the calculation of the circular dichroism electronic spectrum, and of the optical rotation as well. I the case of the complex frequency z:

$$G(z) = -\frac{c}{3}\sum_n \frac{1}{\Omega_{0n}} \times \left(\frac{R_{0n}}{\mathrm{z} - \Omega_{0n} + i\eta} - \frac{R_{0n}}{\mathrm{z} + \Omega_{0n} + i\eta}\right)$$

Where Ω_{0n} is the excitation energy from the ground state to the $n-th$ excited state, R_{0n} is the rotatory strength, η is a suitable small parameter making $G(z)$ analytical. Eventually, the optical rotation can be calculated as the real part (which means the dispersive part) of $G(z)$ [10]:

$$\mathrm{Re}[G(\omega)] = \frac{2}{\pi}\int_0^\infty d\omega' \frac{\omega \mathrm{Im}[G(\omega')]}{\omega'^2 - \omega^2}$$

Thus, the optical rotation value stems as the integral over of the energy spectrum of the electronic circular dichroism curve, which means a property able to take into an account all the transitions and relevant intensities. OR seems a value well suited for the weighting and comparison of the intrinsic "chirality" of different compounds.

5. Full details of quantum mechanical calculation of OR

Here it follows first the L-cysteine and then the D-penicillamine output of ab-initio DFT calculations of the optical rotation value.

L-cysteine output

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scrdir=/home/gungau/scr/
 Entering Link 1 = /home/gungau/g16/l1.exe PID=     25694.

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 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.

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                 6-May-2019
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 S                     0.71992  -2.04257   0.59973
 N                     2.79559   0.41017  -0.21887
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 Using perturbation frequencies:    0.077318
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6	1	0	3.200495	2.228397	0.256462
7	8	0	0.885744	2.322344	2.135431
8	8	0	2.647805	2.787221	0.843922
9	16	0	0.719919	-2.042575	0.599731
10	7	0	2.795593	0.410172	-0.218865
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14	1	0	1.066574	-2.365990	1.859361

Distance matrix (angstroms):

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2	H	1.752452	0.000000			
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4	H	2.478037	3.642921	2.908743	0.000000	
5	H	3.305763	3.879455	2.262214	1.625728	0.000000
6	H	3.800260	4.199391	2.766438	2.381849	2.760727
7	O	3.168826	2.546231	2.819030	3.929367	4.396392
8	O	3.813262	3.977119	2.912839	3.011926	3.508218
9	S	2.364541	2.431050	2.988619	3.395933	3.114779
10	N	2.781720	3.455333	2.068786	1.014586	1.011542
11	C	2.849820	2.676752	2.105346	2.893299	3.315418
12	C	2.162838	2.162521	1.093359	2.057762	2.056752
13	C	1.091112	1.085456	2.143901	2.644794	2.922816
14	H	3.285979	2.578718	2.800484	4.257346	3.597339

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12	C	2.269239	2.420941	2.415411	2.827343	1.465684
13	C	3.638471	2.867178	3.653501	1.835759	2.540695
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		11	12	13	14
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12	C	1.544530	0.000000		
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14	H	4.402684	3.108492	2.403306	0.000000

Stoichiometry C3H7NO2S
Framework group C1[X(C3H7NO2S)]
Deg. of freedom 36
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

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      4          1           0       -0.061686    1.776428   -1.056186
      5          1           0        0.463475    2.167046    0.431973
      6          1           0       -2.155868    1.401185    0.014703
      7          8           0       -1.826934   -1.563460    0.025005
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     10          7           0       -0.251982    1.654877   -0.067046
     11          6           0       -1.628079   -0.379791    0.070008
     12          6           0       -0.229611    0.235300    0.296999
     13          6           0        0.847650   -0.613800   -0.381760
     14          1           0        2.605785   -0.602629    1.256751
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0.9548688
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 There are   312 symmetry adapted basis functions of A   symmetry.
   312 basis functions,   525 primitive gaussians,   354 cartesian basis
functions
    32 alpha electrons       32 beta electrons
       nuclear repulsion energy       373.2532998700 Hartrees.
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Big=F
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 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 PrsmSu:  requested number of processors reduced to:  16 ShMem   1 Linda.
 NBasis=   312 RedAO= T EigKep=  3.70D-04  NBF=   312
 NBsUse=   312 1.00D-06 EigRej= -1.00D+00 NBFU=   312
 ExpMin= 1.03D-01 ExpMax= 3.74D+05 ExpMxC= 1.18D+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
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NMtDT0=    0
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 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.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
 SCF Done:  E(RB3LYP) =  -722.098887128     A.U. after   13 cycles
            NFock= 13  Conv=0.68D-08     -V/T= 2.0045
 DoSCS=F DFT=T ScalE2(SS,OS)=  1.000000  1.000000
 Range of M.O.s used for correlation:     1   312
 NBasis=   312 NAE=    32 NBE=    32 NFC=     0 NFV=     0
 NROrb=    312 NOA=    32 NOB=    32 NVA=   280 NVB=   280
          Differentiating once with respect to magnetic field using GIAOs.
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NMtDT0=    0
 Symmetry not used in FoFCou.
 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.
 CalDSu exits because no D1Ps are significant.
          There are     3 degrees of freedom in the 1st order CPHF.
IDoFFX=0 NUNeed=     3.
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1.92D+01 1.19D+00.
 AX will form     3 AO Fock derivatives at one time.
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1.12D+00 2.65D-01.
      3 vectors produced by pass  2 Test12= 5.97D-13 3.33D-08 XBig12= 6.07D-
01 2.63D-01.
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01 1.11D-01.
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02 2.13D-02.
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07 1.39D-04.
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08 2.94D-05.
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11 1.28D-06.
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 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)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                 (A) (A) (A) (A) (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 --  -88.90171 -19.17019 -19.11548 -14.34312 -
10.30720
 Alpha  occ. eigenvalues --  -10.24546 -10.22591  -7.95383  -5.91835  -
5.91487
 Alpha  occ. eigenvalues --   -5.90888  -1.10727  -1.02681  -0.93132  -
0.80789
 Alpha  occ. eigenvalues --   -0.72976  -0.64657  -0.60505  -0.56052  -
0.51611
 Alpha  occ. eigenvalues --   -0.49380  -0.46530  -0.45837  -0.43678  -
0.42088
 Alpha  occ. eigenvalues --   -0.40147  -0.38162  -0.34503  -0.32399  -
0.31045
 Alpha  occ. eigenvalues --   -0.27795  -0.25797
 Alpha virt. eigenvalues --   -0.01741   0.00579   0.02460   0.03086
0.04694
 Alpha virt. eigenvalues --    0.07197   0.08546   0.09341   0.10506
0.16332
 Alpha virt. eigenvalues --    0.17272   0.19259   0.20849   0.22103
0.24101
```

```
 Alpha virt. eigenvalues --    0.24941   0.26946   0.27805   0.28619
0.29383
 Alpha virt. eigenvalues --    0.30518   0.31010   0.34044   0.34678
0.36029
 Alpha virt. eigenvalues --    0.38232   0.39428   0.40581   0.41736
0.42706
 Alpha virt. eigenvalues --    0.43081   0.43150   0.45191   0.46545
0.49059
 Alpha virt. eigenvalues --    0.50459   0.51629   0.53495   0.54588
0.55753
 Alpha virt. eigenvalues --    0.57685   0.61139   0.62259   0.64022
0.65084
 Alpha virt. eigenvalues --    0.67123   0.67934   0.70364   0.72478
0.75200
 Alpha virt. eigenvalues --    0.76830   0.80298   0.80852   0.81331
0.82334
 Alpha virt. eigenvalues --    0.85796   0.87197   0.88442   0.91217
0.93323
 Alpha virt. eigenvalues --    0.94190   0.97946   0.98834   1.03088
1.06587
 Alpha virt. eigenvalues --    1.08073   1.09145   1.10226   1.11326
1.13046
 Alpha virt. eigenvalues --    1.15859   1.17596   1.20185   1.21707
1.23422
 Alpha virt. eigenvalues --    1.25024   1.26435   1.28482   1.31146
1.32630
 Alpha virt. eigenvalues --    1.33229   1.34550   1.37517   1.40694
1.41215
 Alpha virt. eigenvalues --    1.45597   1.48987   1.51396   1.53967
1.55797
 Alpha virt. eigenvalues --    1.58041   1.59573   1.60478   1.62228
1.63835
 Alpha virt. eigenvalues --    1.65921   1.66958   1.70722   1.71757
1.74239
 Alpha virt. eigenvalues --    1.76391   1.78013   1.79945   1.81629
1.83369
 Alpha virt. eigenvalues --    1.87549   1.90320   1.94712   1.98360
1.99205
 Alpha virt. eigenvalues --    2.01724   2.05167   2.09358   2.11822
2.13969
 Alpha virt. eigenvalues --    2.15023   2.16244   2.19181   2.26090
2.27020
 Alpha virt. eigenvalues --    2.33943   2.38631   2.40012   2.43720
2.45477
 Alpha virt. eigenvalues --    2.51671   2.52525   2.52617   2.58680
2.59653
 Alpha virt. eigenvalues --    2.62554   2.66890   2.68309   2.70759
2.73199
 Alpha virt. eigenvalues --    2.75450   2.79745   2.84993   2.85716
2.88112
 Alpha virt. eigenvalues --    2.90515   2.93160   2.95066   2.99728
3.01684
 Alpha virt. eigenvalues --    3.03948   3.04387   3.06645   3.07626
3.11052
 Alpha virt. eigenvalues --    3.12262   3.14191   3.15423   3.18095
3.19886
 Alpha virt. eigenvalues --    3.22357   3.24415   3.26976   3.27579
3.30816
 Alpha virt. eigenvalues --    3.31309   3.31768   3.33904   3.34450
3.38666
```

```
 Alpha virt. eigenvalues --    3.39878   3.42200   3.44722   3.45793
3.46142
 Alpha virt. eigenvalues --    3.49730   3.50604   3.52479   3.54143
3.56107
 Alpha virt. eigenvalues --    3.61177   3.62160   3.63279   3.66040
3.69853
 Alpha virt. eigenvalues --    3.70838   3.72272   3.73288   3.76077
3.77684
 Alpha virt. eigenvalues --    3.81474   3.82816   3.86340   3.88231
3.90872
 Alpha virt. eigenvalues --    3.92336   3.95792   3.97734   3.99918
4.01486
 Alpha virt. eigenvalues --    4.02252   4.03585   4.06562   4.07717
4.08801
 Alpha virt. eigenvalues --    4.10159   4.13142   4.13492   4.16537
4.18605
 Alpha virt. eigenvalues --    4.20855   4.23823   4.25275   4.28610
4.28860
 Alpha virt. eigenvalues --    4.33205   4.35513   4.38548   4.41056
4.43051
 Alpha virt. eigenvalues --    4.45048   4.48251   4.49479   4.56807
4.63670
 Alpha virt. eigenvalues --    4.66275   4.72400   4.75612   4.81253
4.89623
 Alpha virt. eigenvalues --    4.91659   4.95110   4.98161   4.98277
5.03560
 Alpha virt. eigenvalues --    5.06997   5.10726   5.14319   5.17642
5.18256
 Alpha virt. eigenvalues --    5.21346   5.24282   5.28650   5.34355
5.35184
 Alpha virt. eigenvalues --    5.38919   5.39398   5.52268   5.57843
5.62172
 Alpha virt. eigenvalues --    5.63866   5.64853   5.69367   5.73649
5.77337
 Alpha virt. eigenvalues --    5.87100   5.89664   5.93482   5.94058
5.98319
 Alpha virt. eigenvalues --    6.10311   6.17786   6.26351   6.31541
6.33688
 Alpha virt. eigenvalues --    6.41749   6.44716   6.62169   6.63721
6.70750
 Alpha virt. eigenvalues --    6.77444   6.81487   6.84334   6.91218
6.98087
 Alpha virt. eigenvalues --    7.04685   7.12699   7.34691   7.35928
9.11167
 Alpha virt. eigenvalues --   11.29130  12.04947  12.22589  12.89439
13.16674
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  H    0.573651  -0.021834   0.006544   0.006493  -0.000394  -0.000116
     2  H   -0.021834   0.533052  -0.002215   0.000366  -0.000119  -0.000593
     3  H    0.006544  -0.002215   0.557850   0.007989  -0.010478   0.000145
     4  H    0.006493   0.000366   0.007989   0.558816  -0.042217  -0.003572
     5  H   -0.000394  -0.000119  -0.010478  -0.042217   0.541664  -0.001520
     6  H   -0.000116  -0.000593   0.000145  -0.003572  -0.001520   0.458342
     7  O    0.001279   0.017394  -0.000361  -0.000144  -0.000310   0.005537
     8  O    0.000219   0.000814  -0.000348   0.002362   0.000005   0.312529
     9  S   -0.032547  -0.027054  -0.000882   0.001735   0.011861  -0.000144
    10  N   -0.003560   0.007159  -0.028062   0.383606   0.373731   0.068801
    11  C   -0.000453   0.008354  -0.011441   0.005456   0.001905  -0.049180
    12  C   -0.041391  -0.044622   0.383461  -0.049840  -0.020901  -0.005839
```

```
    13  C    0.398044   0.395729  -0.026331  -0.008884  -0.004260   0.003610
    14  H    0.004219  -0.005857   0.003404   0.000142  -0.000074  -0.000018
                7          8          9         10         11         12
     1  H    0.001279   0.000219  -0.032547  -0.003560  -0.000453  -0.041391
     2  H    0.017394   0.000814  -0.027054   0.007159   0.008354  -0.044622
     3  H   -0.000361  -0.000348  -0.000882  -0.028062  -0.011441   0.383461
     4  H   -0.000144   0.002362   0.001735   0.383606   0.005456  -0.049840
     5  H   -0.000310   0.000005   0.011861   0.373731   0.001905  -0.020901
     6  H    0.005537   0.312529  -0.000144   0.068801  -0.049180  -0.005839
     7  O    7.672795  -0.090235   0.000131   0.002662   0.804514  -0.126568
     8  O   -0.090235   7.678918  -0.000285  -0.026402   0.462297  -0.111702
     9  S    0.000131  -0.000285  15.646645   0.000288   0.002633  -0.056433
    10  N    0.002662  -0.026402   0.000288   6.377640  -0.030013   0.269936
    11  C    0.804514   0.462297   0.002633  -0.030013   4.400321   0.170825
    12  C   -0.126568  -0.111702  -0.056433   0.269936   0.170825   5.388278
    13  C    0.007090   0.004991   0.265088  -0.067764  -0.051742   0.300894
    14  H   -0.000018   0.000002   0.348223   0.000188  -0.000142  -0.003947
               13         14
     1  H    0.398044   0.004219
     2  H    0.395729  -0.005857
     3  H   -0.026331   0.003404
4  H   -0.008884   0.000142
     5  H   -0.004260  -0.000074
     6  H    0.003610  -0.000018
     7  O    0.007090  -0.000018
     8  O    0.004991   0.000002
     9  S    0.265088   0.348223
    10  N   -0.067764   0.000188
    11  C   -0.051742  -0.000142
    12  C    0.300894  -0.003947
    13  C    4.989105  -0.023032
14  H   -0.023032   0.585309
 Mulliken charges:
               1
     1  H    0.109848
     2  H    0.139426
     3  H    0.120725
     4  H    0.137694
     5  H    0.151108
     6  H    0.212017
     7  O   -0.293766
     8  O   -0.233164
     9  S   -0.159258
    10  N   -0.328210
    11  C    0.286666
    12  C   -0.052150
    13  C   -0.182538
    14  H    0.091603
 Sum of Mulliken charges =  -0.00000
 Mulliken charges with hydrogens summed into heavy atoms:
               1
     7  O   -0.293766
     8  O   -0.021147
     9  S   -0.067655
    10  N   -0.039408
    11  C    0.286666
    12  C    0.068575
    13  C    0.066736
 Electronic spatial extent (au):  <R**2>=           1139.3654
 Charge=              0.0000 electrons
```

```
 Dipole moment (field-independent basis, Debye):
    X=              2.4699    Y=              2.8310    Z=
0.3996  Tot=              3.7782
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=            -62.3375   YY=            -50.9578   ZZ=            -
44.8445
   XY=             -4.7490   XZ=              2.0010   YZ=             -
1.5135
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=             -9.6242   YY=              1.7555   ZZ=
7.8688
   XY=             -4.7490   XZ=              2.0010   YZ=             -
1.5135
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=             -0.2394  YYY=             14.1066  ZZZ=             -
0.2651  XYY=              3.2084
  XXY=             10.1152  XXZ=              9.0415  XZZ=             -
1.3087  YZZ=              1.8123
  YYZ=             -0.7450  XYZ=             -1.9209
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=          -1164.9267 YYYY=           -301.6824 ZZZZ=            -
77.8043 XXXY=            -13.1860
 XXXZ=             25.1786 YYYX=            -10.0998 YYYZ=             -
2.9495 ZZZX=              3.6916
 ZZZY=             -4.9092 XXYY=           -242.4811 XXZZ=           -
181.9334 YYZZ=            -59.9493
 XXYZ=             -7.2808 YYXZ=              3.4421 ZZXY=             -
0.4591
N-N= 3.732532998700D+02 E-N=-2.450843018753D+03  KE= 7.188854621202D+02
 AllDun F.D. properties on file 20721 Mask=       2 NFrqRd=     1 NDeriv=
1 ND12= 1 LenFil=      12:
 Frequencies=    0.077318
 Property number 2 -- FD Optical Rotation Tensor frequency  1    0.077318:
                 1             2             3
      1   0.119446D+02 -0.140591D+02  0.209370D+02
      2  -0.297995D+01  0.907161D+00  0.855331D-01
      3  -0.125776D+02  0.872783D+01 -0.148988D+02
 1\1\GINC-GUNDAM\SP\RB3LYP\CC-pVTZ\C3H7N1O2S1\GUNGAU\06-May-2019\0\\# B
 3LYP/cc-pVTZ polar=optrot cphf=rdfreq\\Title Card Required\\0,1\H,0,0.
 035736,0.140123,0.000752\H,0,-0.013888,-0.02736,1.744476\H,0,2.501899,
 0.037838,1.794835\H,0,2.244093,0.493845,-1.06635\H,0,3.271448,-0.48108
 8,-0.268202\H,0,3.200495,2.228397,0.256462\O,0,0.885744,2.322344,2.135
 431\O,0,2.647805,2.787221,0.843922\S,0,0.719919,-2.042575,0.599731\N,0
 ,2.795593,0.410172,-0.218865\C,0,1.744307,1.957594,1.378815\C,0,1.9395
 43,0.481358,0.968712\C,0,0.588902,-0.230815,0.865008\H,0,1.066574,-2.3
 6599,1.859361\\Version=EM64L-G16RevB.01\State=1-A\HF=-722.0988871\RMSD
=6.750e-09\Dipole=0.650835,-1.1203082,-0.7286066\Quadrupole=2.2241433,
 -6.1552457,3.9311024,-1.082875,0.7658375,-5.3485774\PG=C01 [X(C3H7N1O2
S1)]\\@


 THE WHOLE OF SCIENCE IS NOTHING MORE THAN A REFINEMENT OF EVERYDAY THINK-
ING.
                                                          -- A. EINSTEIN
 Job cpu time:       0 days  2 hours 20 minutes 15.5 seconds.
 Elapsed time:       0 days  0 hours  7 minutes 49.0 seconds.
 File lengths (MBytes):  RWF=     59 Int=      0 D2E=      0 Chk=      8
Scr=      1
 Normal termination of Gaussian 16 at Mon May  6 15:55:34 2019.
```

D-penicillamine output

```
Entering Gaussian System, Link 0=g09
 Initial command:
 /home/gungau/g16/l1.exe /home/gungau/scr/Gau-25058.inp -
scrdir=/home/gungau/scr/
 Entering Link 1 = /home/gungau/g16/l1.exe PID=     25060.

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```

```
 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:  EM64L-G16RevB.01 20-Dec-2017
                6-May-2019
 ****************************************
 %chk=D-penicillamineOptRot.chk
 %mem=1GB
 %nprocshared=24
 Will use up to   24 processors via shared memory.
 ----------------------------------------------------------------
 # B3LYP/cc-pVTZ polar=optrot cphf=rdfreq geom=check guess=read
 ----------------------------------------------------------------
 1/29=2,38=1,83=21,172=1/1;
 2/12=2,40=1/2;
 3/5=16,6=1,11=2,14=-4,25=1,30=1,36=2,74=-5,116=-2/1,2,3;
 4/5=1/1;
 5/5=2,38=6,98=1/2;
 8/6=4,10=90,11=11/1;
 10/6=1,13=10,46=8,60=-2,72=3/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 99/5=1,9=1/99;
 -------------------
 Title Card Required
 -------------------
 Structure from the checkpoint file:  "L-penicillamineOptRot.chk"
 Charge =  0 Multiplicity = 1
 No Z-Matrix found in chk file; cartesian coordinates used.
  C                                                  2.390375691253    -
0.723107428881      0.410592587221
  C                                                  1.567563242063
1.191340826100     -0.997531460357
  H                                                  4.243438966937
1.041102777118      1.237284465085
  H                                                  4.373691317325
1.395483733070     -1.662299520573
  H                                                  4.668178772317    -
0.044348286467     -0.911676031209
  H                                                  4.014494918147
4.380518875940      1.429083920175
  O                                                  3.664187090512
3.577599463570     -0.687585852352
  O                                                  4.046639805793
3.415555092326      1.517258895441
```

```
  S                                                  1.468751597096
1.507047410990      1.776089867103
  N                                                  4.656528277452
0.958586864414     -0.794643440837
  C                                                  3.816697544493
2.898642483976      0.295415716407
  C                                                  3.793814217159
1.373920345822      0.301833930900
  C                                                  2.328588521806
0.801586932089      0.270739504274
  H                                                  0.303335907052
0.867399790099      1.570728022033
  H                                                  2.880031240866     -
1.175548958627     -0.455195781048
  H                                                  1.385386580315     -
1.141448585209      0.463729820814
  H                                                  2.926175079090     -
1.018915892131      1.311854668947
  H                                                  0.564811747519
0.763837201587     -0.978755159667
  H                                                  2.074012924159
0.797597545792     -1.881658128170
  H                                                  1.480296558644
2.269149808422     -1.105267024187
 Recover connectivity data from disk.
 Using perturbation frequencies:    0.077318
                         Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        2.390376   -0.723107    0.410593
      2          6           0        1.567563    1.191341   -0.997531
      3          1           0        4.243439    1.041103    1.237284
      4          1           0        4.373691    1.395484   -1.662300
      5          1           0        4.668179   -0.044348   -0.911676
      6          1           0        4.014495    4.380519    1.429084
      7          8           0        3.664187    3.577599   -0.687586
      8          8           0        4.046640    3.415555    1.517259
      9         16           0        1.468752    1.507047    1.776090
     10          7           0        4.656528    0.958587   -0.794643
     11          6           0        3.816698    2.898642    0.295416
     12          6           0        3.793814    1.373920    0.301834
     13          6           0        2.328589    0.801587    0.270740
     14          1           0        0.303336    0.867400    1.570728
     15          1           0        2.880031   -1.175549   -0.455196
     16          1           0        1.385387   -1.141449    0.463730
     17          1           0        2.926175   -1.018916    1.311855
     18          1           0        0.564812    0.763837   -0.978755
     19          1           0        2.074013    0.797598   -1.881658
     20          1           0        1.480297    2.269150   -1.105267
 ---------------------------------------------------------------------
                  Distance matrix (angstroms):
                      1          2          3          4          5
    1  C    0.000000
    2  C    2.514944   0.000000
    3  H    2.688810   3.489597   0.000000
    4  H    3.566350   2.891011   2.924062   0.000000
    5  H    2.719834   3.338879   2.444717   1.650235   0.000000
    6  H    5.451797   4.695401   3.352745   4.312321   5.048357
```

7	O	4.617864	3.191571	3.236429	2.493009	3.765199
8	O	4.593087	4.173382	2.398987	3.781169	4.272817
9	S	2.772646	2.793279	2.864665	4.502626	4.457269
10	N	3.068572	3.104359	2.075134	1.011782	1.009808
11	C	3.894192	3.105672	2.125954	2.530292	3.292914
12	C	2.525667	2.584159	1.089953	2.048058	2.061215
13	C	1.532341	1.529568	2.158293	2.876073	2.754523
14	H	2.869035	2.880827	3.958001	5.224857	5.103476
15	H	1.092728	2.760230	3.104338	3.209101	2.164593
16	H	1.089879	2.758692	3.678367	4.459371	3.724526
17	H	1.089430	3.473374	2.446308	4.095146	2.988051
18	H	2.733857	1.090240	4.303488	3.920940	4.182736
19	H	2.768942	1.092339	3.807034	2.386233	2.894725
20	H	3.475583	1.086690	3.824997	3.073322	3.943646

		6	7	8	9	10
6	H	0.000000				
7	O	2.290783	0.000000			
8	O	0.969517	2.243628	0.000000		
9	S	3.854615	3.895744	3.217903	0.000000	
10	N	4.131197	2.802754	3.428345	4.131755	0.000000
11	C	1.876242	1.204381	1.346467	3.105122	2.378521
12	C	3.218544	2.419082	2.389446	2.756278	1.455692
13	C	4.122232	3.226214	3.367245	1.871650	2.564955
14	H	5.112218	4.872421	4.528607	1.345183	4.955157
15	H	5.975568	4.823000	5.131256	3.763864	2.797446
16	H	6.191627	5.365433	5.381308	2.956987	4.085832
17	H	5.509272	5.066594	4.578446	2.952980	3.367785
18	H	5.547827	4.196208	5.038335	2.993099	4.100484
19	H	5.250125	3.418022	4.722033	3.774756	2.806582
20	H	4.159685	2.579898	3.844217	2.980462	3.450001

		11	12	13	14	15
11	C	0.000000				
12	C	1.524907	0.000000			
13	C	2.571521	1.573346	0.000000		
14	H	4.253949	3.748346	2.407478	0.000000	
15	H	4.247328	2.812097	2.177186	3.862301	0.000000
16	H	4.718256	3.486232	2.168470	2.536090	1.754865
17	H	4.144085	2.738358	2.180656	3.241063	1.774579
18	H	4.093369	3.526835	2.161844	2.564948	3.065220
19	H	3.491560	2.838574	2.167404	3.880611	2.564716
20	H	2.795880	2.851970	2.183285	3.242081	3.774626

		16	17	18	19	20
16	H	0.000000				
17	H	1.763054	0.000000			
18	H	2.526701	3.741810	0.000000		
19	H	3.120088	3.771528	1.758995	0.000000	
20	H	3.755388	4.329482	1.766376	1.766564	0.000000

Stoichiometry C5H11NO2S
Framework group C1[X(C5H11NO2S)]
Deg. of freedom 54
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.077946	0.907713	-0.707863
2	6	0	-0.979898	0.660207	1.541131

```
      3          1           0        0.344471    0.231449   -1.658791
      4          1           0        1.053351    2.291715    0.291320
      5          1           0        0.057808    2.566992   -0.995688
      6          1           0        2.706351   -1.659068   -0.213671
      7          8           0        2.133705    0.172461    1.037436
      8          8           0        1.984413   -1.235571   -0.702975
      9         16           0       -1.145064   -1.621906   -0.061084
     10          7           0        0.796410    1.979665   -0.636208
     11          6           0        1.595589   -0.164173    0.013891
     12          6           0        0.424049    0.572435   -0.626612
     13          6           0       -0.944220    0.234133    0.072537
     14          1           0       -2.350973   -1.664429    0.533468
     15          1           0       -2.000963    1.996075   -0.647876
     16          1           0       -3.045144    0.632455   -0.287630
     17          1           0       -2.070081    0.612024   -1.756369
     18          1           0       -1.948383    0.416254    1.978334
     19          1           0       -0.845399    1.740789    1.627485
     20          1           0       -0.205282    0.171566    2.126020
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           1.6969364           1.2060705
0.9383638
 Standard basis: CC-pVTZ (5D, 7F)
 There are   484 symmetry adapted cartesian basis functions of A   symmetry.
 There are   428 symmetry adapted basis functions of A   symmetry.
   428 basis functions,   697 primitive gaussians,   484 cartesian basis
functions
    40 alpha electrons       40 beta electrons
       nuclear repulsion energy       584.2606457902 Hartrees.
 NAtoms=   20 NActive=   20 NUniq=   20 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.
 PrsmSu:  requested number of processors reduced to:  16 ShMem   1 Linda.
 NBasis=   428 RedAO= T EigKep=  2.68D-04  NBF=   428
 NBsUse=   428 1.00D-06 EigRej= -1.00D+00 NBFU=   428
 Initial guess from the checkpoint file:  "L-penicillamineOptRot.chk"
 B after Tr=    -0.000000    0.000000   -0.000000
         Rot=    1.000000   -0.000000   -0.000000    0.000000 Ang=   0.00
deg.
 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.
 SCF Done:  E(RB3LYP) =  -800.746843814     A.U. after   12 cycles
            NFock= 12  Conv=0.56D-08     -V/T= 2.0048
 DoSCS=F DFT=T ScalE2(SS,OS)=  1.000000  1.000000
 Range of M.O.s used for correlation:     1   428
 NBasis=   428 NAE=    40 NBE=    40 NFC=     0 NFV=     0
 NROrb=    428 NOA=    40 NOB=    40 NVA=   388 NVB=   388

 **** Warning!!: The largest alpha MO coefficient is  0.12207552D+02

          Differentiating once with respect to magnetic field using GIAOs.
          Electric field/nuclear overlap derivatives assumed to be zero.
 PrsmSu:  requested number of processors reduced to:  14 ShMem   1 Linda.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
         NFxFlg=           0 DoJE=F BraDBF=F KetDBF=T FulRan=T
```

```
         wScrn=  0.000000 ICntrl=      6100 IOpCl=  0 I1Cent=           7
NGrid=          20
         NMat0=    1 NMatS0=      1 NMatT0=    0 NMatD0=    1 NMtDS0=    0
NMtDT0=    0
 Symmetry not used in FoFCou.
 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.
 CalDSu exits because no D1Ps are significant.
          There are     3 degrees of freedom in the 1st order CPHF.
IDoFFX=0 NUNeed=     3.
      3 vectors produced by pass  0 Test12= 1.03D-12 3.33D-08 XBig12=
2.17D+01 9.76D-01.
 AX will form     3 AO Fock derivatives at one time.
      3 vectors produced by pass  1 Test12= 1.03D-12 3.33D-08 XBig12= 8.44D-
01 3.74D-01.
      3 vectors produced by pass  2 Test12= 1.03D-12 3.33D-08 XBig12= 4.66D-
01 2.66D-01.
      3 vectors produced by pass  3 Test12= 1.03D-12 3.33D-08 XBig12= 1.51D-
01 7.98D-02.
      3 vectors produced by pass  4 Test12= 1.03D-12 3.33D-08 XBig12= 3.95D-
02 3.04D-02.
      3 vectors produced by pass  5 Test12= 1.03D-12 3.33D-08 XBig12= 4.55D-
03 1.24D-02.
      3 vectors produced by pass  6 Test12= 1.03D-12 3.33D-08 XBig12= 1.39D-
03 5.07D-03.
      3 vectors produced by pass  7 Test12= 1.03D-12 3.33D-08 XBig12= 1.27D-
04 1.93D-03.
      3 vectors produced by pass  8 Test12= 1.03D-12 3.33D-08 XBig12= 1.84D-
05 6.86D-04.
      3 vectors produced by pass  9 Test12= 1.03D-12 3.33D-08 XBig12= 2.74D-
06 3.31D-04.
      3 vectors produced by pass 10 Test12= 1.03D-12 3.33D-08 XBig12= 2.12D-
07 7.88D-05.
      3 vectors produced by pass 11 Test12= 1.03D-12 3.33D-08 XBig12= 1.12D-
08 1.79D-05.
      3 vectors produced by pass 12 Test12= 1.03D-12 3.33D-08 XBig12= 6.04D-
10 3.82D-06.
      3 vectors produced by pass 13 Test12= 1.03D-12 3.33D-08 XBig12= 2.05D-
11 9.45D-07.
      3 vectors produced by pass 14 Test12= 1.03D-12 3.33D-08 XBig12= 7.87D-
13 1.96D-07.
      1 vectors produced by pass 15 Test12= 1.03D-12 3.33D-08 XBig12= 2.17D-
14 3.90D-08.
 InvSVY:  IOpt=1 It=  1 EMax= 4.44D-16
 Solved reduced A of dimension    46 with     3 vectors.
 Dipole-magnetic dipole polarizability for W=    0.077318:
                 1             2             3
      1  -0.287798D+00 -0.191465D+01 -0.924447D+01
      2   0.970756D+01  0.457455D+01 -0.249792D+02
      3   0.161904D+02  0.322537D+02 -0.300842D+01
 w=    0.077318 a.u., Optical Rotation Beta=     -0.4261 au.
 Molar Mass =    149.2074 grams/mole, [Alpha] ( 5893.0 A) =     -110.38 deg.
 End of Minotr F.D. properties on file   721 Mask=       2 NFrqRd=     1
NDeriv=     1 ND12= 1 LenFil=      12:
 Frequencies=    0.077318
 Property number 2 -- FD Optical Rotation Tensor frequency  1    0.077318:
                 1             2             3
      1  -0.287798D+00 -0.191465D+01 -0.924447D+01
```

```
      2   0.970756D+01  0.457455D+01 -0.249792D+02
      3   0.161904D+02  0.322537D+02 -0.300842D+01
 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)
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                 (A) (A) (A) (A)
       Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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                 (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 --  -88.88460 -19.18541 -19.12696 -14.31218 -
10.31520
 Alpha  occ. eigenvalues --  -10.23593 -10.23259 -10.18129 -10.17285  -
7.93696
 Alpha  occ. eigenvalues --   -5.90143  -5.89805  -5.89195  -1.12063  -
1.03132
 Alpha  occ. eigenvalues --   -0.91161  -0.82840  -0.72900  -0.71047  -
0.70540
 Alpha  occ. eigenvalues --   -0.62392  -0.56306  -0.53702  -0.49924  -
0.49169
```

```
 Alpha  occ. eigenvalues --   -0.46613  -0.46201  -0.44412  -0.43248  -
0.42086
 Alpha  occ. eigenvalues --   -0.40262  -0.39675  -0.38740  -0.36977  -
0.36305
 Alpha  occ. eigenvalues --   -0.33385  -0.31999  -0.29194  -0.25732  -
0.24556
 Alpha virt. eigenvalues --   -0.00943   0.00395   0.02448   0.03645
0.04301
 Alpha virt. eigenvalues --    0.06653   0.07927   0.08447   0.10117
0.10830
 Alpha virt. eigenvalues --    0.12538   0.13569   0.14962   0.15283
0.16482
 Alpha virt. eigenvalues --    0.18140   0.18634   0.19625   0.22668
0.23281
 Alpha virt. eigenvalues --    0.24368   0.26119   0.26786   0.27244
0.28572
 Alpha virt. eigenvalues --    0.30388   0.30981   0.31490   0.33223
0.34322
 Alpha virt. eigenvalues --    0.35398   0.35955   0.38011   0.38988
0.39453
 Alpha virt. eigenvalues --    0.40869   0.41469   0.42907   0.43286
0.44382
 Alpha virt. eigenvalues --    0.44876   0.45466   0.45559   0.46733
0.47484
 Alpha virt. eigenvalues --    0.48062   0.49515   0.50223   0.50768
0.52414
 Alpha virt. eigenvalues --    0.53032   0.53434   0.54395   0.56447
0.57644
 Alpha virt. eigenvalues --    0.58032   0.58989   0.60336   0.62501
0.65309
 Alpha virt. eigenvalues --    0.67158   0.68089   0.69881   0.71103
0.72966
 Alpha virt. eigenvalues --    0.73611   0.76107   0.76981   0.80066
0.81098
 Alpha virt. eigenvalues --    0.82957   0.83647   0.85385   0.85883
0.87754
 Alpha virt. eigenvalues --    0.89167   0.90681   0.93114   0.93580
0.94331
 Alpha virt. eigenvalues --    0.95589   0.97378   0.98412   1.00100
1.01309
 Alpha virt. eigenvalues --    1.02028   1.02418   1.03492   1.04137
1.07043
 Alpha virt. eigenvalues --    1.08062   1.10509   1.12374   1.12993
1.14138
 Alpha virt. eigenvalues --    1.16657   1.17223   1.19270   1.19765
1.21616
 Alpha virt. eigenvalues --    1.22650   1.23678   1.25159   1.25988
1.27433
 Alpha virt. eigenvalues --    1.28419   1.28962   1.29391   1.30641
1.31425
 Alpha virt. eigenvalues --    1.32592   1.33580   1.35302   1.35603
1.38767
 Alpha virt. eigenvalues --    1.40589   1.43241   1.43713   1.45504
1.48402
 Alpha virt. eigenvalues --    1.49304   1.50989   1.51843   1.53100
1.54813
 Alpha virt. eigenvalues --    1.55382   1.58373   1.59533   1.62194
1.62907
 Alpha virt. eigenvalues --    1.63287   1.65849   1.67371   1.68634
1.70439
```

```
 Alpha virt. eigenvalues --    1.73272   1.74081   1.74814   1.77064
1.81098
 Alpha virt. eigenvalues --    1.81576   1.84181   1.86926   1.89606
1.90952
 Alpha virt. eigenvalues --    1.93478   1.94691   1.97346   1.98243
2.01849
 Alpha virt. eigenvalues --    2.03435   2.05308   2.06840   2.11450
2.15161
 Alpha virt. eigenvalues --    2.16235   2.18682   2.24950   2.28405
2.29520
 Alpha virt. eigenvalues --    2.32164   2.34295   2.35294   2.39321
2.41011
 Alpha virt. eigenvalues --    2.42370   2.44593   2.45722   2.50439
2.51594
 Alpha virt. eigenvalues --    2.52926   2.55040   2.58073   2.58986
2.61428
 Alpha virt. eigenvalues --    2.62182   2.64823   2.66168   2.68732
2.71870
 Alpha virt. eigenvalues --    2.72480   2.73812   2.77602   2.79627
2.80232
 Alpha virt. eigenvalues --    2.80997   2.82336   2.84895   2.85967
2.88098
 Alpha virt. eigenvalues --    2.90736   2.92004   2.92886   2.94188
2.95869
 Alpha virt. eigenvalues --    2.97201   2.99260   3.00775   3.02113
3.03308
 Alpha virt. eigenvalues --    3.04369   3.05141   3.05908   3.08325
3.09426
 Alpha virt. eigenvalues --    3.10829   3.11238   3.12557   3.13520
3.15667
 Alpha virt. eigenvalues --    3.17702   3.18876   3.20440   3.21690
3.22575
 Alpha virt. eigenvalues --    3.23986   3.25198   3.27343   3.30807
3.31231
 Alpha virt. eigenvalues --    3.33376   3.34758   3.35276   3.35568
3.36894
 Alpha virt. eigenvalues --    3.37738   3.38825   3.39645   3.40650
3.42748
 Alpha virt. eigenvalues --    3.43151   3.43998   3.44614   3.46916
3.47417
 Alpha virt. eigenvalues --    3.49192   3.51180   3.52695   3.53651
3.55049
 Alpha virt. eigenvalues --    3.56867   3.58087   3.59464   3.61353
3.62039
 Alpha virt. eigenvalues --    3.62927   3.64664   3.65213   3.67710
3.68627
 Alpha virt. eigenvalues --    3.69733   3.71323   3.73969   3.75876
3.76619
 Alpha virt. eigenvalues --    3.79494   3.80368   3.81549   3.83749
3.85316
 Alpha virt. eigenvalues --    3.86758   3.87982   3.89515   3.91824
3.94709
 Alpha virt. eigenvalues --    3.95810   3.97277   3.98591   3.98961
4.00765
 Alpha virt. eigenvalues --    4.03366   4.05158   4.05711   4.06486
4.06818
 Alpha virt. eigenvalues --    4.08651   4.09902   4.11402   4.13334
4.14075
 Alpha virt. eigenvalues --    4.14760   4.16615   4.16918   4.18471
4.19329
```

```
 Alpha virt. eigenvalues --    4.19658   4.20385   4.23369   4.24417
4.25364
 Alpha virt. eigenvalues --    4.28287   4.28769   4.30586   4.32036
4.33818
 Alpha virt. eigenvalues --    4.34861   4.35905   4.39559   4.40848
4.41854
 Alpha virt. eigenvalues --    4.44516   4.46660   4.50368   4.53365
4.56799
 Alpha virt. eigenvalues --    4.57749   4.61342   4.64884   4.65373
4.68422
 Alpha virt. eigenvalues --    4.71964   4.79443   4.80787   4.81744
4.85604
 Alpha virt. eigenvalues --    4.86129   4.87705   4.89753   4.93281
4.95642
 Alpha virt. eigenvalues --    4.99386   5.02055   5.04488   5.06733
5.11233
 Alpha virt. eigenvalues --    5.14450   5.15164   5.15954   5.17676
5.19091
 Alpha virt. eigenvalues --    5.20235   5.21519   5.22153   5.25349
5.26036
 Alpha virt. eigenvalues --    5.26552   5.31449   5.34431   5.35770
5.37231
 Alpha virt. eigenvalues --    5.39771   5.40611   5.42078   5.44804
5.49999
 Alpha virt. eigenvalues --    5.51887   5.54077   5.59663   5.64224
5.70881
 Alpha virt. eigenvalues --    5.74224   5.75451   5.77803   5.91016
5.92562
 Alpha virt. eigenvalues --    5.93071   5.94564   5.95721   5.96215
6.01904
 Alpha virt. eigenvalues --    6.10892   6.15011   6.19218   6.24303
6.30541
 Alpha virt. eigenvalues --    6.36715   6.41879   6.45596   6.52773
6.58883
 Alpha virt. eigenvalues --    6.66671   6.75894   6.78074   6.87106
6.88866
 Alpha virt. eigenvalues --    6.89902   7.02592   7.20355   7.29827
7.42958
 Alpha virt. eigenvalues --    9.20700   9.50194  11.91753  12.35661
13.20631
 Alpha virt. eigenvalues --   13.29739  13.65740  13.75171
          Condensed to atoms (all electrons):
               1          2          3          4          5          6
     1  C    4.972794  -0.051551  -0.006715  -0.001398   0.002132   0.000111
     2  C   -0.051551   4.970021   0.008435   0.003415  -0.002001  -0.000064
     3  H   -0.006715   0.008435   0.519113   0.005628  -0.007374  -0.001130
     4  H   -0.001398   0.003415   0.005628   0.530049  -0.052811  -0.000249
     5  H    0.002132  -0.002001  -0.007374  -0.052811   0.550906   0.000076
     6  H    0.000111  -0.000064  -0.001130  -0.000249   0.000076   0.472656
     7  O   -0.000420   0.004755   0.003024   0.019051  -0.000316   0.010510
     8  O   -0.000289   0.000276   0.008703   0.000798  -0.000240   0.324688
     9  S   -0.057690  -0.058267  -0.001429  -0.000023  -0.000000   0.000921
    10  N   -0.000693   0.003922  -0.014839   0.401880   0.399211  -0.000774
    11  C    0.000779  -0.002470  -0.018526  -0.006822   0.007118  -0.041183
    12  C   -0.052040  -0.056480   0.404857  -0.046690  -0.033176   0.020763
    13  C    0.321169   0.301549  -0.038510  -0.003003  -0.002105  -0.001059
    14  H   -0.009651  -0.010224  -0.000118   0.000011   0.000009  -0.000024
    15  H    0.385282  -0.005515   0.000243   0.000410   0.003185   0.000001
    16  H    0.397759  -0.005378   0.000046   0.000033  -0.000116  -0.000004
    17  H    0.399505   0.008383   0.003681   0.000041   0.000428   0.000007
```

18	H	-0.007425	0.397374	-0.000221	0.000230	-0.000121	-0.000021
19	H	-0.003849	0.382091	-0.000300	0.001318	0.001288	0.000037
20	H	0.008636	0.396105	-0.000083	-0.000317	-0.000073	0.000093
		7	8	9	10	11	12
1	C	-0.000420	-0.000289	-0.057690	-0.000693	0.000779	-0.052040
2	C	0.004755	0.000276	-0.058267	0.003922	-0.002470	-0.056480
3	H	0.003024	0.008703	-0.001429	-0.014839	-0.018526	0.404857
4	H	0.019051	0.000798	-0.000023	0.401880	-0.006822	-0.046690
5	H	-0.000316	-0.000240	-0.000000	0.399211	0.007118	-0.033176
6	H	0.010510	0.324688	0.000921	-0.000774	-0.041183	0.020763
7	O	7.737789	-0.095753	-0.001716	-0.004608	0.755275	-0.111733
8	O	-0.095753	7.636462	0.001956	0.001638	0.454904	-0.084618
9	S	-0.001716	0.001956	15.671460	0.003859	0.004853	-0.037655
10	N	-0.004608	0.001638	0.003859	6.337253	-0.023877	0.320439
11	C	0.755275	0.454904	0.004853	-0.023877	4.368426	0.218513
12	C	-0.111733	-0.084618	-0.037655	0.320439	0.218513	5.137727
13	C	-0.005093	-0.001854	0.280516	-0.106144	-0.021354	0.314669
14	H	-0.000050	0.000299	0.340316	-0.000309	0.000023	0.003718
15	H	-0.000010	0.000001	0.010748	0.008620	-0.000270	-0.008073
16	H	0.000009	0.000002	-0.002873	0.000182	-0.000210	0.007278
17	H	0.000000	-0.000085	0.002236	0.000017	0.000262	-0.001586
18	H	0.000547	-0.000001	-0.002537	-0.000028	0.000160	0.006516
19	H	-0.001983	-0.000059	0.010383	0.017672	0.000041	-0.009801
20	H	0.008858	-0.000486	0.001557	-0.001232	0.000600	-0.001385
		13	14	15	16	17	18
1	C	0.321169	-0.009651	0.385282	0.397759	0.399505	-0.007425
2	C	0.301549	-0.010224	-0.005515	-0.005378	0.008383	0.397374
3	H	-0.038510	-0.000118	0.000243	0.000046	0.003681	-0.000221
4	H	-0.003003	0.000011	0.000410	0.000033	0.000041	0.000230
5	H	-0.002105	0.000009	0.003185	-0.000116	0.000428	-0.000121
6	H	-0.001059	-0.000024	0.000001	-0.000004	0.000007	-0.000021
7	O	-0.005093	-0.000050	-0.000010	0.000009	0.000000	0.000547
8	O	-0.001854	0.000299	0.000001	0.000002	-0.000085	-0.000001
9	S	0.280516	0.340316	0.010748	-0.002873	0.002236	-0.002537
10	N	-0.106144	-0.000309	0.008620	0.000182	0.000017	-0.000028
11	C	-0.021354	0.000023	-0.000270	-0.000210	0.000262	0.000160
12	C	0.314669	0.003718	-0.008073	0.007278	-0.001586	0.006516
13	C	5.143488	-0.009621	-0.040682	-0.030555	-0.034028	-0.031974
14	H	-0.009621	0.599938	-0.000273	0.002965	-0.000689	0.002359
15	H	-0.040682	-0.000273	0.619686	-0.029288	-0.029422	-0.000571
16	H	-0.030555	0.002965	-0.029288	0.579643	-0.024759	0.003927
17	H	-0.034028	-0.000689	-0.029422	-0.024759	0.565947	-0.000062
18	H	-0.031974	0.002359	-0.000571	0.003927	-0.000062	0.595231
19	H	-0.044338	-0.000383	0.003610	-0.000539	-0.000275	-0.032877
20	H	-0.024019	-0.000792	-0.000449	-0.000200	-0.000407	-0.026118
		19	20				
1	C	-0.003849	0.008636				
2	C	0.382091	0.396105				
3	H	-0.000300	-0.000083				
4	H	0.001318	-0.000317				
5	H	0.001288	-0.000073				
6	H	0.000037	0.000093				
7	O	-0.001983	0.008858				
8	O	-0.000059	-0.000486				
9	S	0.010383	0.001557				
10	N	0.017672	-0.001232				
11	C	0.000041	0.000600				
12	C	-0.009801	-0.001385				
13	C	-0.044338	-0.024019				
14	H	-0.000383	-0.000792				

```
    15  H    0.003610  -0.000449
    16  H   -0.000539  -0.000200
    17  H   -0.000275  -0.000407
    18  H   -0.032877  -0.026118
    19  H    0.624287  -0.025836
    20  H   -0.025836   0.542754
 Mulliken charges:
1
     1  C   -0.296445
     2  C   -0.284378
     3  H    0.135512
     4  H    0.148449
     5  H    0.133979
     6  H    0.214645
     7  O   -0.318136
     8  O   -0.246345
     9  S   -0.166615
    10  N   -0.342191
    11  C    0.303760
    12  C    0.008758
    13  C    0.032949
    14  H    0.082494
    15  H    0.082766
    16  H    0.102076
    17  H    0.110804
    18  H    0.095611
    19  H    0.079514
    20  H    0.122792
 Sum of Mulliken charges =  -0.00000
 Mulliken charges with hydrogens summed into heavy atoms:
               1
     1  C   -0.000799
     2  C    0.013539
     7  O   -0.318136
     8  O   -0.031700
     9  S   -0.084121
    10  N   -0.059763
    11  C    0.303760
    12  C    0.144270
    13  C    0.032949
 Electronic spatial extent (au):  <R**2>=           1404.2002
 Charge=             -0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=             -1.8735    Y=              0.8026    Z=             -
0.1088  Tot=              2.0411
 Quadrupole moment (field-independent basis, Debye-Ang):
XX=            -60.4111   YY=            -60.7081   ZZ=            -66.0792
   XY=             -6.2628   XZ=             -2.2979   YZ=             -
1.0267
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX=              1.9884   YY=              1.6913   ZZ=             -3.6797
   XY=             -6.2628   XZ=             -2.2979   YZ=             -
1.0267
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=             14.2031  YYY=              5.4700  ZZZ=             -
2.6171  XYY=              8.7833
  XXY=            -22.4153  XXZ=             -0.2122  XZZ=             -
2.6020  YZZ=              1.5401
  YYZ=              5.1792  XYZ=              4.9134
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
```

```
 XXXX=           -838.7805 YYYY=           -568.6887 ZZZZ=           -
323.3117 XXXY=            -45.4214
 XXXZ=            -26.1349 YYYX=            -26.8849 YYYZ=
2.7514 ZZZX=              0.6021
ZZZY=             -0.7613 XXYY=           -226.1547 XXZZ=           -
222.5269 YYZZ=           -163.2932
 XXYZ=             -3.9456 YYXZ=              9.5287 ZZXY=             -
6.0419
 N-N= 5.842606457902D+02 E-N=-3.054793176630D+03  KE= 7.969459184387D+02
AllDun F.D. properties on file 20721 Mask=       2 NFrqRd=     1 NDeriv=
1 ND12= 1 LenFil=      12:
 Frequencies=    0.077318
 Property number 2 -- FD Optical Rotation Tensor frequency  1    0.077318:
1             2             3
      1  -0.305340D+01 -0.141196D+01  0.251569D+02
      2   0.310917D+01 -0.179694D+01 -0.103962D+02
      3  -0.357354D+02  0.775001D+01  0.612868D+01
 1\1\GINC-GUNDAM\SP\RB3LYP\CC-pVTZ\C5H11N1O2S1\GUNGAU\06-May-2019\0\\#
 B3LYP/cc-pVTZ polar=optrot cphf=rdfreq geom=check guess=read\\Title Ca
 rd Required\\0,1\C,2.3903756913,-0.7231074289,0.4105925872\C,1.5675632
 421,1.1913408261,-0.9975314604\H,4.2434389669,1.0411027771,1.237284465
1\H,4.3736913173,1.3954837331,-1.6622995206\H,4.6681787723,-0.04434828
 65,-0.9116760312\H,4.0144949181,4.3805188759,1.4290839202\O,3.66418709
 05,3.5775994636,-0.6875858524\O,4.0466398058,3.4155550923,1.5172588954
 \S,1.4687515971,1.507047411,1.7760898671\N,4.6565282775,0.9585868644,-
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 3739203458,0.3018339309\C,2.3285885218,0.8015869321,0.2707395043\H,0.3
033359071,0.8673997901,1.570728022\H,2.8800312409,-1.1755489586,-0.455
 195781\H,1.3853865803,-1.1414485852,0.4637298208\H,2.9261750791,-1.018
 9158921,1.3118546689\H,0.5648117475,0.7638372016,-0.9787551597\H,2.074
 0129242,0.7975975458,-1.8816581282\H,1.4802965586,2.2691498084,-1.1052
 670242\\Version=EM64L-G16RevB.01\State=1-A\HF=-800.7468438\RMSD=5.588e
-09\Dipole=-0.306207,-0.7327932,-0.1186961\Quadrupole=-1.0559094,3.352
 5634,-2.2966541,1.0685449,1.2744919,4.3848122\PG=C01 [X(C5H11N1O2S1)]\
\@


 ERWIN WITH HIS PSI CAN DO
 CALCULATIONS QUITE A FEW.
 BUT ONE THING HAS NOT BEEN SEEN
 JUST WHAT DOES PSI REALLY MEAN.
 -- WALTER HUCKEL, TRANS. BY FELIX BLOCH
 Job cpu time:       0 days  8 hours 49 minutes 43.7 seconds.
 Elapsed time:       0 days  0 hours 23 minutes 36.7 seconds.
 File lengths (MBytes):  RWF=    132 Int=      0 D2E=      0 Chk=    160
Scr=      1
 Normal termination of Gaussian 16 at Mon May  6 15:39:02 2019.
```

References

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