

# The Calculation of X-ray Scattering Factors for Spherically Averaged Molecules

## Example: Methane, CH<sub>4</sub>

All molecular gas-phases become crystalline when subjected to sufficient pressure. It seems that the lowest pressure phases may be characterized as close-packed structures wherein each molecule is freely rotating about an associated point. As pressure is increased the motion is constrained and a lowering of symmetry occurs. In order to model the freely rotating molecule, the molecular electron-density wave functions were computed using the *Gaussian92* program for energy-optimized model molecules. The electron-density was then spherically averaged in order to mimic the rotations. The Fourier transform of this spherically averaged electron density provides the scattering factor for the rotating molecule. Displacement parameters obtained from the structure refinements provide estimates of translational motion.

A general outline of the procedure is as follows:

- 1) Find the minimum energy structure of CH<sub>4</sub> using the Gaussian code.
- 2) Calculate the molecular orbital coefficients for this configuration.
- 3) Calculate the spherically averaged electron density for the molecule.
- 4) Transform the electron density into scattering factors.

### The Minimum Energy Structure of CH<sub>4</sub>

The structure of CH<sub>4</sub> was calculated using *the Gaussian 92 for Windows* code assuming tetrahedral symmetry with a high level 6-31G\*\* basis set and MP2 Møller-Plesset configuration interactions. The length of the CH bond was varied (optimized at 1.0855 Å) until a minimum energy (-40.3646259 a.u.) was obtained. The optimized bond length compares well with a reported CD bond length of 1.084 Å for solid heavy methane at 34.5 K (Press, 1972).

## Molecular Orbital Coefficients

A single point calculation was then carried out at the minimum energy configuration in order to obtain the molecular orbital coefficients. A brief review of the form of the basis sets is now given. See Szabo and Ostlund (1982) for a more complete description.

Consider an expansion of a molecular orbital,  $\psi_i$ ,

$$\psi_i = \sum_{\mu=1}^K C_{\mu i} \phi_{\mu},$$

where  $C_{\mu i}$  are the expansion coefficients and  $\phi_{\mu}$  are previously prescribed linear combinations (or contractions) of Gaussian functions (primitives). The contraction has the form

$$\phi_{\mu}(\mathbf{r} - \mathbf{R}_A) = \sum_{p=1}^L d_{p\mu} g_p(\alpha_{p\mu}, \mathbf{r} - \mathbf{R}_A),$$

where  $\alpha_{p\mu}$  and  $d_{p\mu}$  are the contraction exponents and coefficients,  $L$  is the length of the contraction, and  $\mathbf{R}_A$  is the position of the center of the atom A. The normalized Gaussian primitives are of the forms

$$g_{1s}(\alpha, \mathbf{r}) = (8\alpha^3/\pi^3)^{1/4} e^{-\alpha r^2}$$

$$g_{2p_x}(\alpha, \mathbf{r}) = (128\alpha^5/\pi^3)^{1/4} x e^{-\alpha r^2}$$

$$g_{3d_{xx}}(\alpha, \mathbf{r}) = (2048\alpha^7/9\pi^3)^{1/4} xy e^{-\alpha r^2}$$

$$g_{3d_{xy}}(\alpha, \mathbf{r}) = (2048\alpha^7/\pi^3)^{1/4} xy e^{-\alpha r^2}.$$

The contraction coefficients ( $d$ 's) and exponents ( $\alpha$ 's) are obtained by a least-squares fit which, for the 1s shell, minimizes the integral

$$\int d\mathbf{r} [\phi_{1s}^{SF}(\mathbf{r}) - \phi_{1s}^{CGF}(\mathbf{r})]^2,$$

and for the higher order  $s$  and  $p$  shells, minimizes the integral

$$\int d\mathbf{r} [\phi_s^{SF}(\mathbf{r}) - \phi_s^{CGF}(\mathbf{r})]^2 + \int d\mathbf{r} [\phi_p^{SF}(\mathbf{r}) - \phi_p^{CGF}(\mathbf{r})]^2.$$

This means that the contractions for higher order  $s$  and  $p$  shells have the same radial behavior because they share the same exponents and thus are treated as  $sp$  functions. This is done in order to save computing time.  $\phi^{SF}$  and  $\phi^{CGF}$  represent Slater functions and contracted Gaussian functions, respectively.

In this study I used a 6-31G\*\* basis set. The 6-31G part of the acronym means that for the carbon atom the inner shell functions are a contraction of 6 primitive Gaussians and the outer valence shell functions are split into a contraction of 3 primitives and 1 primitive Gaussian. The first \*, 6-31G\*, means that an uncontracted d-type polarization function is also included for carbon. Hydrogen does not have an inner shell, its functions are simply a contraction of 3 primitive Gaussians and 1 primitive Gaussian. The second \*, 6-31G\*\*, means that there is also an uncontracted p-type polarization function included for hydrogen. An example of the basis sets is given below. The first column are the exponents ( $\alpha$ 's) and in the second column are the contraction coefficients ( $d$ 's). For the  $sp$  functions, the first column contains the exponents and the second and third columns contain the contraction coefficients for the  $s$  and the  $p$  functions, respectively.

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6-31G\* Basis set for carbon that consists of 4 contractions.

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```

S      6 1.00
  0.3047524880D+04  0.1834737130D-02
  0.4573695180D+03  0.1403732280D-01
  0.1039486850D+03  0.6884262220D-01
  0.2921015530D+02  0.2321844430D+00
  0.9286662960D+01  0.4679413480D+00
  0.3163926960D+01  0.3623119850D+00
SP     3 1.00
  0.7868272350D+01 -0.1193324200D+00  0.6899906660D-01
  0.1881288540D+01 -0.1608541520D+00  0.3164239610D+00
  0.5442492580D+00  0.1143456440D+01  0.7443082910D+00
SP     1 1.00
  0.1687144782D+00  0.1000000000D+01  0.1000000000D+01
D      1 1.00
  0.8000000000D+00  0.1000000000D+01

```

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---

6-31G\*\* Basis set for hydrogen that consists of 3 contractions.

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```
S    3 1.00
  0.1873113696D+02  0.3349460434D-01
  0.2825394365D+01  0.2347269535D+00
  0.6401216923D+00  0.8137573262D+00
S    1 1.00
  0.1612777588D+00  0.1000000000D+01
P    1 1.00
  0.1100000000D+01  0.1000000000D+01
```

---

Molecular orbital coefficients are calculated by the Gaussian program and output to a file in a form like the following.

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CH<sub>4</sub> coefficients for occupied molecular orbitals

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EIGENVALUES --				(A1)--0	(A1)--0	(T2)--0	(T2)--0	(T2)--0
				-11.20680	-0.94379	-0.54434	-0.54434	-0.54434
1	1	C	1S	0.99569	-0.19504	0.00000	0.00000	0.00000
2			2S	0.02809	0.36481	0.00000	0.00000	0.00000
3			2PX	0.00000	0.00000	0.16673	0.08239	0.38706
4			2PY	0.00000	0.00000	0.38776	-0.11790	-0.14194
5			2PZ	0.00000	0.00000	0.07903	0.40462	-0.12017
6			3S	-0.01324	0.34649	0.00000	0.00000	0.00000
7			3PX	0.00000	0.00000	0.08255	0.04079	0.19164
8			3PY	0.00000	0.00000	0.19198	-0.05837	-0.07028
9			3PZ	0.00000	0.00000	0.03913	0.20033	-0.05950
10			XX	-0.00178	-0.00116	0.00000	0.00000	0.00000
11			YY	-0.00178	-0.00116	0.00000	0.00000	0.00000
12			ZZ	-0.00178	-0.00116	0.00000	0.00000	0.00000
13			XY	0.00000	0.00000	0.00550	0.02817	-0.00837
14			XZ	0.00000	0.00000	0.02700	-0.00821	-0.00988
15			YZ	0.00000	0.00000	0.01161	0.00574	0.02695
16	2	H	1S	-0.00003	0.13789	0.25095	0.14621	0.04949
17			2S	0.00242	0.04459	0.22038	0.12840	0.04346
18			PX	0.00011	-0.00769	-0.00688	-0.00425	0.00442
19			PY	0.00011	-0.00769	-0.00328	-0.00751	-0.00421
20			PZ	0.00011	-0.00769	-0.00831	0.00100	-0.00385
21	3	H	1S	-0.00003	0.13789	-0.18834	0.17434	-0.14470
22			2S	0.00242	0.04459	-0.16539	0.15310	-0.12707
23			PX	-0.00011	0.00769	-0.00448	0.00801	0.00077
24			PY	-0.00011	0.00769	-0.00088	0.00475	-0.00785
25			PZ	0.00011	-0.00769	0.00849	-0.00007	0.00357
26	4	H	1S	-0.00003	0.13789	0.05624	-0.23961	-0.16194
27			2S	0.00242	0.04459	0.04939	-0.21042	-0.14221
28			PX	-0.00011	0.00769	0.00487	-0.00782	0.00012
29			PY	0.00011	-0.00769	0.00417	0.00724	0.00388
30			PZ	-0.00011	0.00769	0.00344	-0.00257	-0.00815
31	5	H	1S	-0.00003	0.13789	-0.11886	-0.08094	0.25715
32			2S	0.00242	0.04459	-0.10438	-0.07108	0.22582
33			PX	0.00011	-0.00769	0.00726	0.00444	-0.00353
34			PY	-0.00011	0.00769	0.00177	-0.00502	0.00752
35			PZ	-0.00011	0.00769	-0.00326	0.00350	0.00788

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Spherically Averaged Electron Density

If we have an  $N$  electron closed-shell molecule described by a single determinant wave function with each molecular orbital  $\psi_a$  containing two electrons, then the total

charge density at the point  $\mathbf{r}$  is

$$\rho(\mathbf{r}) = 2 \sum_a^{N/2} |\psi_a(\mathbf{r})|^2,$$

where  $\rho(\mathbf{r}) d\mathbf{r}$  is the probability of finding an electron in the volume element  $d\mathbf{r}$  at  $\mathbf{r}$ .

Note that the integral over all space is the total number of electrons,

$$\int \rho(\mathbf{r}) d\mathbf{r} = 2 \sum_a^{N/2} \int |\psi_a(\mathbf{r})|^2 = 2 \sum_a^{N/2} 1 = N.$$

Inserting our expansion of a molecular orbital into the density expression gives

$$\begin{aligned} \rho(\mathbf{r}) &= 2 \sum_a^{N/2} \phi_a^*(\mathbf{r}) \psi_a(\mathbf{r}) \\ &= 2 \sum_a^{N/2} \sum_\nu C_{\nu a}^* \phi_\nu^*(\mathbf{r}) \sum_\mu C_{\mu a} \phi_\mu(\mathbf{r}) \\ &= \sum_{\nu\mu} \left[ 2 \sum_a^{N/2} C_{\nu a}^* C_{\mu a} \right] \phi_\nu^*(\mathbf{r}) \phi_\mu(\mathbf{r}) \\ &= \sum_{\nu\mu} P_{\nu\mu} \phi_\nu^*(\mathbf{r}) \phi_\mu(\mathbf{r}) \\ &= \Phi^* P \Phi \end{aligned}$$

where the density matrix is defined as

$$P_{\nu\mu} = 2 \sum_a^{N/2} C_{\nu a}^* C_{\mu a}$$

and  $\Phi$  is a vector of components,  $\phi_\nu(\mathbf{r})$ . This is the equation that I used to calculate the electron density.

Initially, in order to compute the spherically averaged electron density, calculations were undertaken over a  $90 \times 180$  angular grid (16,200 points for each value of  $r$ ) that covered a complete sphere around the molecule at a series of fixed radii,  $0.000 \leq r \leq 8.000$  bohr, at increments of 0.001 bohr. The spherically averaged electron density at a given value of  $r$  was then computed as

$$\langle \rho(r) \rangle = \frac{\int_0^{2\pi} \int_0^\pi \psi^2(\mathbf{r}) r^2 \sin \phi d\phi d\theta}{\int_0^{2\pi} \int_0^\pi r^2 \sin \phi d\phi d\theta} \approx \frac{1}{4\pi} \sum \rho(\mathbf{r}) \sin \phi \Delta\phi \Delta\theta,$$

where  $\Delta\phi = \pi/89$  and  $\Delta\theta = 2\pi/179$ . A table of 8001  $r$  versus  $\langle \rho(r) \rangle$  data points was constructed.

While this method is theoretically sound, in practice it has its problems. The solution converges very slowly and takes an amazingly long time to compute. When summed over all space the total number of electrons exceeds the true value. This was not really a problem with methane but it was quite apparent with  $H_2$ , probably resulting from its apparent lack of spherical symmetry.

What I ended up doing was to obtain  $\langle \rho(r) \rangle$ , ( $0 \leq r \leq 5\text{\AA}$ ), at intervals of  $0.01\text{\AA}$ . At each value of  $r$  the average electron density was computed from a  $1^\circ \times 1^\circ$  grid using a 10 step Gaussian quadrature method both in  $\phi$  and in  $\theta$ . The results were much more satisfying.

Figure 1 is a plot of the electron density minus the spherically averaged electron density along the CH vector. The difference demonstrates the build up of electron density along the CH vector due to covalent bonding effects. Note that the peak is located near  $r = 0.58\text{\AA}$ . This is where the electron density from the hydrogen atoms is concentrated, even though the hydrogen nuclei are at  $1.0855\text{\AA}$  from the carbon.

#### Scattering Factors

The scattering factor for an atom or a molecule is difficult to calculate unless the electron density demonstrates spherical symmetry. However, with the assumption of spherical electron density,  $\langle \rho(r) \rangle$ , and with the carbon at the origin, then the scattering factor of methane,  $f(s)$ , is the Fourier transform of  $\rho(r)$ ,

$$f(s) = \int_0^\infty U(r) \frac{\sin(2\pi r r^*)}{2\pi r r^*} dr \approx \sum_r U(r) \frac{\sin(2\pi r r^*)}{2\pi r r^*} \Delta r,$$

where  $r^* = 1/d = 2 \sin \theta / \lambda = 2s$  and  $U(r) = 4\pi r^2 \langle \rho(r) \rangle$  is the radial distribution function for methane, as plotted in Figure 2. Note that the first peak represent the electrons from the 1s orbital of C while the second peak is due primarily to electrons in the higher order shells. The hydrogen nuclei are located near the mid-point of the second peak. The scattering factors for 201 values of  $s$ ,  $0.00 \leq s \leq 2.00$ , at  $0.01$

increments were computed and tabulated. The scattering factor curve is presented in Figure 3 and compared to that of carbon.

The last step in the process is to fit the curve to the standard equation that gives an analytical approximation to the scattering factor,

$$f(s) = \sum_{i=1}^4 a_i \exp(-b_i s^2) + c, \quad 0 \leq s \leq 2\text{\AA}^{-1}$$

where  $a_i$  and  $b_i$  are the 8 parameters that are varied and  $c$  is obtained from the constraint

$$c = f(0) - \sum a_i.$$

The fitting procedure was accomplished with a minimization program written by M.B. Boisen Jr. and L.W. Johnson (Boisen and Gibbs, 1993) that is based on a quasi-Newton method that uses a model trust region (with a double dogleg) and the BFGS update (Dennis and Schnabel, 1983). The values of the fitted parameters are

$a$	$b$	$c$
1.543827	0.580871	0.215499
-0.514127	3.995349	
6.180872	13.797434	
2.573929	36.110548	

The quantity that was minimized was the error in the fit, defined by Doyle and Turner (1968) as

$$E = \frac{100}{f(0)} \left[ \frac{\sum_{i=1}^{201} \delta_i^2}{201} \right]^{1/2} = .0185,$$

where  $\delta = f(s)_{\text{actual}} - f(s)_{\text{fitted}}$ . The maximum deviation between actual and fitted values of  $f(s)$  is 0.005.

## References

- Boisen, M.B., Jr. and Gibbs, G.V. (1993) A modeling of the structure and compressibility of quartz with a molecular potential and its transferability to cristobalite and coesite. *Physics and Chemistry of Minerals*, 20, 123-135.
- Dennis, J.E., Jr. and Schnabel, R.B. (1983) *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*. Prentice-Hall, Englewood Cliffs, pp 378.
- Doyle, P.A. and Turner, P.S. (1968) Relativistic Hartree-Fock X-ray and electron scattering factors. *Acta Crystallographica*, A24, 390-397.
- Press, W. (1972) Structure and phase transitions of solid heavy methane (CD<sub>4</sub>). *The Journal of Chemical Physics*, 56, 2597-2609.
- Szabo, A. and Ostlund, H.S. (1982) *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*. MacMillan Publishing Co., Inc, New York.

#MP2/6.31G\*\* Pop=Reg FOpt

methane optimization

0 1

C

H1 C CH

H2 C CH H1 tet

H3 C CH H1 tet H2 120.

H4 C CH H1 tet H2 -120.

CH = 1.08549799

tet = 109.471220634

Entering Link 1 = L1-EXE PID= 2718.  
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 M. Head-Gordon, F. M. W. Gill, M. W. Wong, J. B. Foresman,  
 B. G. Johnson, H. B. Schlegel, M. A. Robb, E. S. Replogle,  
 R. Gomperts, J. L. Andres, K. Raghavachari, J. S. Binkley,  
 C. Gonzalez, R. L. Martin, D. J. Fox, D. J. Defrees, J. Baker,  
 J. J. P. Stewart, and J. A. Pople, Gaussian, Inc.,  
 Pittsburgh PA, 1992.

\*\*\*\*\*  
 Gaussian 92: 486-Windows-C92RevD.2 11-Feb-1993  
 27-Jan-1995  
 \*\*\*\*\*

```

#MP2/6-31G** Pop=Reg Fopt
-----
1/10=7.29=10000/1.3;
2/12=2.14=103/2;
3/5=1.6=6,7=101,11=9,25=20,30=1/1,2,3,11,20;
4//1;
5/5=1/2;
8/6=4,10=1/1;
9/15=2,16=-3/6;
10/5=1/2;
7/12=2,29=1/1,2,3,16;
6//1;
1/10=7/3(1);
99/799;
2//2;
3/5=1,6=6,7=101,11=9,25=20,30=1/1,2,3,11,20;
4/5=5,16=2/1;
5/5=1/2;
8/6=4,10=1/1;
    
```

```

9/15=2,16=-3/6;
10/5=1/2;
7/12=2/1,2,3,16;
1//3(-8);
3/5=1,6=6,7=101,11=9,30=1,39=1/1,1,3;
6//1;
99//99;
-----
methane single point calculation
-----
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
    
```

```

C      C      CH
H1     C      CH
H2     C      CH
H3     C      CH
H4     C      CH
      Variables:
      CH      1.0844
      Constants:
      tet      109.47122
      3 tetrahedral angles replaced.
    
```

```

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
-----
!      Name      Value      Derivative information (Atomic Units)
!      CH      1.0844      estimate D2E/DX2
!      tet      109.4712      Frozen
-----
Initial trust radius is 3.000D-01
Number of steps in this run= 20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
    
```

```

!      Initial Parameters
!      (Angstroms and Degrees)
-----
!      Name      Value      Derivative information (Atomic Units)
!      CH      1.0844      estimate D2E/DX2
!      tet      109.4712      Frozen
-----
Initial trust radius is 3.000D-01
Number of steps in this run= 20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
    
```

```

CD Cent Atom N1 Length/X N2 Alpha/Y N3 Beta/Z
1 1 C 0.000000 0.000000 0.000000 0.000000
2 2 H 1.084400( 1) 2 109.471( 5)
3 3 H 1.084400( 2) 2 109.471( 6) 3 120.000( 8) 0
4 4 H 1.084400( 3) 2 109.471( 7) 3 120.000( 9) 0
5 5 H 1.084400( 4) 2 109.471( 7) 3 120.000( 9) 0
-----
C-Matrix orientation:
-----
Coordinates (Angstroms) 2
Center Atomic X Y Z
Number Number
1 6 0.000000 0.000000 0.000000 0.000000
2 1 0.000000 0.000000 0.000000 1.084400
3 3 1.022382 0.000000 -0.361467
4 1 -0.511191 -0.885409 -0.361467
5 1 -0.511191 0.885409 -0.361467
-----
Distance matrix (angstroms):
2
1 2 3 4 5
1 C 0.000000
2 H 1.084400 0.000000
3 H 1.084400 1.770818 0.000000
4 H 1.084400 1.770818 1.770818 0.000000
5 H 1.084400 1.770818 1.770818 0.000000
-----
Interatomic angles:
H2-C1-H3=109.4712 H3-C1-H4=109.4712
H2-C1-H5=109.4712 H3-C1-H5=109.4712
STOICHIOMETRY CH4
FRAMEWORK GROUP TD[0(C),4C3(H)]
1
DEG. OF FREEDOM
    
```

```

FULL POINT GROUP          TD          NOP 24
LARGEST ABELIAN SUBGROUP D2          NOP 4
LARGEST CONCISE ABELIAN SUBGROUP D2  NOP 4
Standard orientation:
-----
Center   Atomic   Coordinates (Angstroms)
Number   Number      X           Y           Z
-----
1        6          0.000000    0.000000    0.000000
2        1          0.626079    0.626079    0.626079
3        1          0.626079   -0.626079    0.626079
4        1          -0.626079    0.626079   -0.626079
5        1          0.626079   -0.626079   -0.626079
-----
Rotational constants (GHz): 159.9132172 159.9132172 159.9132172
Isotopes: C-12,H-1,H-1,H-1,H-1
Standard basis: 6-31G(D,P) (S, S=P, 6D, 7F)
There are 11 symmetry adapted basis functions of A symmetry.
There are 8 symmetry adapted basis functions of B1 symmetry.
There are 8 symmetry adapted basis functions of B2 symmetry.
There are 8 symmetry adapted basis functions of B3 symmetry.
Crude estimate of integral set expansion from redundant integrals=1.110.
Integral buffers will be 8192 words long.
Two-electron integral symmetry is turned on.
Raffenetti 1 integral format.
35 basis functions
5 alpha electrons
5 beta electrons
nuclear repulsion energy 13.5047725390 Hartrees.
One-electron integrals computed using PRISM.
The smallest eigenvalue of the overlap matrix is 1.743D-02
DipDirv: will hold 34 matrices at once.
Out2e will use a cutoff of 1.00D-10
24933 integrals produced for a total of 24933.
Out2e will use a cutoff of 1.00D-10
27036 integrals produced for a total of 51969.
Projected INDO Guess.
Initial guess orbital symmetries:
Occupied (A1) (A1) (T2) (T2) (T2) (T2) (T2) (T2) (A1) (T2) (A1) (T2)
Virtual (T2) (T2) (T2) (T2) (T2) (T2) (T2) (T2) (2A) (2A) (2A)
(2B) (2B) (2B) (2C) (2C) (2C) (2C) (2C) (2C) (2C) (2C)
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
SCF Done: E(RHF) = -40.2017027643 A.U. after 9 cycles
Convrg = 0.7863D-09 -V/T = 2.0006
S**2 = 0.0000
Range of M.O.s used for correlation: 2 35
NBasis= 35 NAF= 5 NBE= 5 NFC= 1 NFV= 0
NROrb= 34 NOA= 4 NOB= 4 NVA= 30 NVB= 30
Fully direct method.
JobType=1 pass 1: I= 2 to 5.
ANORM= 0.1024944589D+01
E2 = -0.1629202618D+00 EUMP2 = -0.40364623026116D+02
Spin components of T(2) and E(2):
alpha-alpha T2 = 0.479203331D-02 E2= -0.1482189281D-01
alpha-beta T2 = 0.4092680421D-01 E2= -0.1332764782D-00
beta-beta T2 = 0.479203331D-02 E2= -0.1482189281D-01
Differentiating once with respect to electric field.
Differentiating once with respect to dipole field.
Differentiating once with respect to nuclear coordinates.
There are 1 degrees of freedom in the 1st order CPHF.
1 vectors were produced by pass 0.
AX will form 1 AO Fock derivatives at one time.
1 vectors were produced by pass 1.
1 vectors were produced by pass 2.
1 vectors were produced by pass 3.
1 vectors were produced by pass 4.
1 vectors were produced by pass 5.
1 vectors were produced by pass 6.
Inv2: IOpt= 1 Iter= 1 AM= 6.31D-16 Conv= 1.00D-12.
Inverted reduced A of dimensional 7 with in-core refinement.
***** AXES RESTORED TO ORIGINAL SET *****

```

```

Center   Atomic   Forces (Hartrees/Bohr)
Number   Number      X           Y           Z
-----
1        6          0.000000000 0.000000000 0.000000000
2        1          0.000000000 0.000000000 0.000735928
3        1          0.000693839 0.000000000 -0.000245309
4        1          -0.000348920 -0.000600883 -0.000245309
5        1          -0.000348920 0.000600883 -0.000245309
-----
MAX          0.000735928 RMS          0.000380031
Internal Coordinate Forces (Hartree/Bohr or radian)
Cent Atom N1 Length/A N2 Alpha/Y N3 Beta/Z
-----
1 C          0.000736( 1) 0.000000( 5)
2 H          0.000736( 2) 0.000000( 6) 0.000000( 8)
3 H          0.000736( 3) 0.000000( 7) 0.000000( 9)
4 H          0.000736( 4) 0.000000( 7) 0.000000( 9)
5 H          0.000736( 4) 0.000000( 7) 0.000000( 9)
-----
MAX          0.000735928 RMS          0.000490619
-----
Population analysis using the SCF density.
-----
Orbital Symmetries.
Occupied (A1) (T2) (T2) (T2) (T2) (T2) (T2) (T2) (T2) (T2) (T2)
Virtual (A1) (A1) (E) (E) (T1) (T1) (T2) (T2) (T2) (T2) (T2)
(T2) (T2) (T2) (E) (E) (A1) (T2) (T2) (T2) (T2) (A1)
The electronic state is 1-A1.
Alpha occ. eigenvalues -- -11.20627 -0.94425 -0.54462 -0.54462 -0.54462
Alpha virt. eigenvalues -- 0.25686 0.32759 0.32759 0.32759 0.72606
Alpha virt. eigenvalues -- 0.72606 0.72606 1.14410 1.14410 1.14410
Alpha virt. eigenvalues -- 1.21285 1.31572 1.62947 1.62947 2.35367
Alpha virt. eigenvalues -- 2.35367 2.35367 2.37694 2.37694 2.37694
Alpha virt. eigenvalues -- 2.96350 2.96350 2.96350 2.96350 2.96350
Alpha virt. eigenvalues -- 3.49900 3.81087 3.81087 3.81087 4.84254
Molecular Orbital Coefficients
-----
EIGENVALUES -- (A1) (T2) (T2) (T2) (T2) (T2) (T2) (T2) (T2) (T2)
1 C          -11.20627 -0.94425 -0.54462 -0.54462 -0.54462
2 S          0.25686 0.32759 0.32759 0.32759 0.72606
3 S          0.72606 0.72606 1.14410 1.14410 1.14410
4 2PX        0.02812 0.36480 0.00000 0.00000 0.00000
5 2PY        0.00000 0.00000 -0.26524 0.12787 0.31283
6 2PZ        0.00000 0.00000 -0.03754 0.38406 -0.18881
7 3S         0.00000 0.00000 0.33586 0.14390 0.22595
8 3PY        0.00000 0.00000 -0.13117 0.06323 0.15470
9 3PZ        0.00000 0.00000 -0.01856 0.18933 0.09337
10 XX        0.00000 0.00000 0.16609 0.07116 0.11174
11 YY        -0.00179 0.09118 0.00000 0.00000 0.00000
12 ZZ        -0.00179 -0.00118 0.00000 0.00000 0.00000
13 XY        0.00000 0.00000 0.00000 0.00000 0.00000
14 XZ        0.00000 0.00000 -0.00261 0.02673 -0.01573
15 YZ        0.00000 0.00000 0.00000 -0.01846 -0.00890
16 2 H 1S    -0.00003 0.13802 0.01310 0.25976 0.13861
17 2 S 2S    0.00243 0.04452 0.01150 0.22786 0.12159
18 PX        0.00010 -0.00765 -0.00493 -0.00784 -0.00019
19 PY        0.00010 -0.00769 -0.00111 -0.00366 -0.00838
20 PZ        0.00010 -0.00769 0.00498 -0.00758 -0.00161
21 3 H 1S    -0.00003 0.13802 0.25295 -0.14577 0.04037
22 2 S 2S    0.00243 0.04452 0.22188 -0.12786 0.03541
23 PX        0.00010 0.00769 0.00534 -0.00348 0.00665
24 PY        0.00010 0.00769 0.00906 0.00070 -0.00154
25 PZ        0.00010 -0.00769 -0.00419 0.00792 0.00215
26 4 H 1S    -0.00003 0.13802 0.13802 -0.28818 -0.00461
27 2 S 2S    0.00243 0.04452 -0.03758 -0.03901 -0.25279

```

