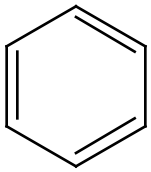
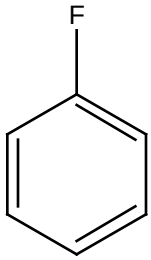
Chemistry 416, Dr. Glaser
Applications of IR/Raman Spectra: Benzene

Attached you will find the printout of an *ab initio* calculation of benzene. The calculation was carried out at the (rather low) RHF/STO-3G level, the same level we used in the calculations of water and ammonia in the previous assignments. By now you should be used to the printout sequence and you should be able to find the pertinent information without help.





(a) Make a drawing of the molecule using the Cartesian coordinates found in the section "Standard Orientation".

(b) Consider the number of frequencies. Calculate the total number of vibrations. How many frequencies are we observing in the IR and in the Raman spectra?

(c) Draw the normal mode representations for each vibration and discuss why each normal mode is active/inactive in the IR/Raman.

(d) Considering your drawings of the normal modes, name these vibrations as "stretching" and "bending" modes and so on and state whether they are "symmetric" or "asymmetric".

(e) Consider the effects of a substitution of one H versus F, fluorobenzene, on the spectra. What do you you expect to change? Compare the number of frequencies and their intensities to the parent benzene.

(1 attachment, freq. calc. of benzene at RHF/STO-3G, edited for brevity).

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****************************************
Gaussian 88:  VAX-VMS-G88RevC  19-Aug-1988
    VAX-3100  VMS-5.2  Sun 26-SEP-1993
****************************************
Default route: RHF/6-31G* Name=GLASER 6D 10F
------------------------------------------
# RHF/Sto-3g guess=read geom=checkpoint freq
------------------------------------------
1/10=4,29=10002,30=1/1,3;
2/10=1,12=2/2;
3/11=1,25=14,30=1/1,2,3,11,14;
4/5=1,7=1/1;
5//1;
8/6=4,11=10/1;
10/8=1,13=10/2;
11/6=2,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,8=1,9=1/2;
7/8=1,10=1,25=1/7,2,3,16;
1/10=4,30=1/3;
6/7=2,8=2,9=2,10=2,18=1/1;
99//99;
------------
benzene freq
------------
   Charge = 0 Multiplicity = 1
Z-Matrix taken from the checkpoint file:
DKB0:[GROUP.GLASER]BENZENE.CHK;1
X
C,1,CX
C,1,CX,2,60.
C,1,CX,3,60.,2,180.,0
C,1,CX,4,60.,3,180.,0
C,1,CX,5,60.,4,180.,0
C,1,CX,6,60.,5,180.,0
X,2,1.,1,90.,3,0.,0
X,3,1.,1,90.,4,0.,0
X,4,1.,1,90.,5,0.,0
X,5,1.,1,90.,6,0.,0
X,6,1.,1,90.,7,0.,0
X,7,1.,1,90.,2,0.,0
H,2,CH,8,90.,1,180.,0
H,3,CH,9,90.,1,180.,0
H,4,CH,10,90.,1,180.,0
H,5,CH,11,90.,1,180.,0
H,6,CH,12,90.,1,180.,0
H,7,CH,13,90.,1,180.,0
     Variables:
CX=1.38676597
CH=1.08263527
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                      ----------------------------
                      !   Initial Parameters    !
                      ! (Angstroms and Degrees) !
---------------------                            ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------
```

```
!       CX          1.3868   calculate D2E/DX2 analytically           !
!       CH          1.0826   calculate D2E/DX2 analytically           !
--------------------------------------------------------------------------
Initial trust radius is 3.000D-01.
Number of steps in this run=  20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
--------------------------------------------------------------------------
                        Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
--------------------------------------------------------------------------
  1      X
  2   1  C     1   1.386766(  1)
  3   2  C     1   1.386766(  2)   2   60.000( 19)
  4   3  C     1   1.386766(  3)   3   60.000( 20)   2  180.000( 36)   0
  5   4  C     1   1.386766(  4)   4   60.000( 21)   3  180.000( 37)   0
  6   5  C     1   1.386766(  5)   5   60.000( 22)   4  180.000( 38)   0
  7   6  C     1   1.386766(  6)   6   60.000( 23)   5  180.000( 39)   0
  8      X     2   1.000000(  7)   1   90.000( 24)   3    0.000( 40)   0
  9      X     3   1.000000(  8)   1   90.000( 25)   4    0.000( 41)   0
 10      X     4   1.000000(  9)   1   90.000( 26)   5    0.000( 42)   0
 11      X     5   1.000000( 10)   1   90.000( 27)   6    0.000( 43)   0
 12      X     6   1.000000( 11)   1   90.000( 28)   7    0.000( 44)   0
 13      X     7   1.000000( 12)   1   90.000( 29)   2    0.000( 45)   0
 14   7  H     2   1.082635( 13)   8   90.000( 30)   1  180.000( 46)   0
 15   8  H     3   1.082635( 14)   9   90.000( 31)   1  180.000( 47)   0
 16   9  H     4   1.082635( 15)  10   90.000( 32)   1  180.000( 48)   0
 17  10  H     5   1.082635( 16)  11   90.000( 33)   1  180.000( 49)   0
 18  11  H     6   1.082635( 17)  12   90.000( 34)   1  180.000( 50)   0
 19  12  H     7   1.082635( 18)  13   90.000( 35)   1  180.000( 51)   0
--------------------------------------------------------------------------
STOICHIOMETRY    C6H6
FRAMEWORK GROUP  D6H[3C2'(HC.CH)]
DEG. OF FREEDOM    2
FULL POINT GROUP                 D6H     NOP 24
LARGEST ABELIAN SUBGROUP         D2H     NOP  8
LARGEST CONCISE ABELIAN SUBGROUP D2      NOP  4
                  Standard orientation:
---------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------
   1          6           0.000000    1.386766    0.000000
   2          6           1.200975    0.693383    0.000000
   3          6           1.200975   -0.693383    0.000000
   4          6           0.000000   -1.386766    0.000000
   5          6          -1.200975   -0.693383    0.000000
   6          6          -1.200975    0.693383    0.000000
   7          1           0.000000    2.469401    0.000000
   8          1           2.138564    1.234701    0.000000
   9          1           2.138564   -1.234701    0.000000
  10          1           0.000000   -2.469401    0.000000
  11          1          -2.138564   -1.234701    0.000000
  12          1          -2.138564    1.234701    0.000000
---------------------------------------------------------------
Rotational constants (GHZ):      5.7646077      5.7646077      2.8823038
Isotopes: C-12,C-12,C-12,C-12,C-12,C-12,H-1,H-1,H-1,H-1,H-1,H-1
Radii and axes of the molecular ellipsoid:
                         1         2         3
```

```
    EIGENVALUES --     5.03149   4.40630   0.76400
        1             -0.86603  -0.50000   1.00000
        2             -0.50000   0.86603   0.00000
        3              0.00000   0.00000   0.00000
Standard basis: STO-3G     (S, S=P, 5D, 7F)
THERE ARE   9 SYMMETRY ADAPTED BASIS FUNCTIONS OF AG  SYMMETRY.
THERE ARE   6 SYMMETRY ADAPTED BASIS FUNCTIONS OF B1G SYMMETRY.
THERE ARE   1 SYMMETRY ADAPTED BASIS FUNCTIONS OF B2G SYMMETRY.
THERE ARE   2 SYMMETRY ADAPTED BASIS FUNCTIONS OF B3G SYMMETRY.
THERE ARE   1 SYMMETRY ADAPTED BASIS FUNCTIONS OF AU  SYMMETRY.
THERE ARE   2 SYMMETRY ADAPTED BASIS FUNCTIONS OF B1U SYMMETRY.
THERE ARE   9 SYMMETRY ADAPTED BASIS FUNCTIONS OF B2U SYMMETRY.
THERE ARE   6 SYMMETRY ADAPTED BASIS FUNCTIONS OF B3U SYMMETRY.
 36 basis functions     108 primitive gaussians
 21 alpha electrons       21 beta electrons
    nuclear repulsion energy  204.5361003939 Hartrees.

                  -227.891360371
                  -227.891360371
                  -227.891360371
                  -227.891360371
SCF DONE:  E(RHF) =  -227.891360371     A.U. AFTER    3 CYCLES
           CONVG  =    0.3768E-13             -V/T =  2.0081
KE= 2.260621385293D+02 PE=-9.399037518418D+02 EE= 2.814141525477D+02
RANGE OF M.O.'S USED FOR CORRELATION:   1  36
Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
Raman scattering activities (A**4/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:
                     1                      2                      3
                   E2U                    E2U                    E2G
Frequencies --   478.0501               478.0501               700.1833
Red. masses --     2.9907                 2.9907                 6.0668
Frc consts  --     0.4027                 0.4027                 1.7524
IR Inten    --     0.0000                 0.0000                 0.0000
Raman Activ --     0.0000                 0.0000                 2.2959
Depolar     --     0.0000                 0.0000                 0.7500
Atom AN      X      Y      Z        X      Y      Z        X      Y      Z
  1   6     0.00   0.00   0.25     0.00   0.00  -0.01     0.15   0.00   0.00
  2   6     0.00   0.00  -0.12     0.00   0.00   0.22     0.23   0.22   0.00
  3   6     0.00   0.00  -0.13     0.00   0.00  -0.21    -0.23   0.22   0.00
  4   6     0.00   0.00   0.25     0.00   0.00  -0.01    -0.15   0.00   0.00
  5   6     0.00   0.00  -0.12     0.00   0.00   0.22    -0.23  -0.22   0.00
  6   6     0.00   0.00  -0.13     0.00   0.00  -0.21     0.23  -0.22   0.00
  7   1     0.00   0.00   0.52     0.00   0.00  -0.01    -0.22   0.00   0.00
  8   1     0.00   0.00  -0.25     0.00   0.00   0.46     0.33   0.06   0.00
  9   1     0.00   0.00  -0.27     0.00   0.00  -0.45    -0.33   0.06   0.00
 10   1     0.00   0.00   0.52     0.00   0.00  -0.01     0.22   0.00   0.00
 11   1     0.00   0.00  -0.25     0.00   0.00   0.46    -0.33  -0.06   0.00
 12   1     0.00   0.00  -0.27     0.00   0.00  -0.45     0.33  -0.06   0.00
                     4                      5                      6
                   E2G                    A2U                    B2G
Frequencies --   700.1833               811.2595               841.2059
Red. masses --     6.0668                 1.0848                 3.6121
Frc consts  --     1.7524                 0.4207                 1.5060
IR Inten    --     0.0000                24.5885                 0.0000
Raman Activ --     2.2959                 0.0000                 0.0000
Depolar     --     0.7500                 0.0000                 0.0000
Atom AN      X      Y      Z        X      Y      Z        X      Y      Z
```

1	6	0.00	0.36	0.00	0.00	0.00	-0.03	0.00	0.00	0.20
2	6	-0.22	0.02	0.00	0.00	0.00	-0.03	0.00	0.00	-0.20
3	6	-0.22	-0.02	0.00	0.00	0.00	-0.03	0.00	0.00	0.20
4	6	0.00	-0.36	0.00	0.00	0.00	-0.03	0.00	0.00	-0.20
5	6	0.22	-0.02	0.00	0.00	0.00	-0.03	0.00	0.00	0.20
6	6	0.22	0.02	0.00	0.00	0.00	-0.03	0.00	0.00	-0.20
7	1	0.00	0.36	0.00	0.00	0.00	0.41	0.00	0.00	0.36
8	1	-0.06	-0.25	0.00	0.00	0.00	0.41	0.00	0.00	-0.36
9	1	-0.06	0.25	0.00	0.00	0.00	0.41	0.00	0.00	0.36
10	1	0.00	-0.36	0.00	0.00	0.00	0.41	0.00	0.00	-0.36
11	1	0.06	0.25	0.00	0.00	0.00	0.41	0.00	0.00	0.36
12	1	0.06	-0.25	0.00	0.00	0.00	0.41	0.00	0.00	-0.36

	7	8	9
	E1G	E1G	B2U
Frequencies --	1037.9420	1037.9420	1154.5115
Red. masses --	1.2483	1.2483	6.8018
Frc consts --	0.7923	0.7923	5.3416
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	6.2116	6.2116	0.0000
Depolar --	0.7500	0.7500	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.09	0.30	0.00	0.00
2	6	0.00	0.00	-0.07	0.00	0.00	0.04	-0.15	0.26	0.00
3	6	0.00	0.00	-0.07	0.00	0.00	-0.04	-0.15	-0.26	0.00
4	6	0.00	0.00	0.00	0.00	0.00	-0.09	0.30	0.00	0.00
5	6	0.00	0.00	0.07	0.00	0.00	-0.04	-0.15	0.26	0.00
6	6	0.00	0.00	0.07	0.00	0.00	0.04	-0.15	-0.26	0.00
7	1	0.00	0.00	0.00	0.00	0.00	-0.57	0.28	0.00	0.00
8	1	0.00	0.00	0.49	0.00	0.00	-0.29	-0.14	0.24	0.00
9	1	0.00	0.00	0.50	0.00	0.00	0.28	-0.14	-0.24	0.00
10	1	0.00	0.00	0.00	0.00	0.00	0.57	0.28	0.00	0.00
11	1	0.00	0.00	-0.49	0.00	0.00	0.29	-0.14	0.24	0.00
12	1	0.00	0.00	-0.50	0.00	0.00	-0.28	-0.14	-0.24	0.00

	10	11	12
	B1U	A1G	E2U
Frequencies --	1156.7288	1172.5077	1190.7667
Red. masses --	6.3996	5.8088	1.3492
Frc consts --	5.0450	4.7051	1.1271
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.0000	36.9452	0.0000
Depolar --	0.0000	0.1023	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.29	0.00	0.00	0.27	0.00	0.00	0.00	-0.10
2	6	-0.25	-0.14	0.00	0.23	0.13	0.00	0.00	0.00	0.05
3	6	0.25	-0.14	0.00	0.23	-0.13	0.00	0.00	0.00	0.05
4	6	0.00	0.29	0.00	0.00	-0.27	0.00	0.00	0.00	-0.10
5	6	-0.25	-0.14	0.00	-0.23	-0.13	0.00	0.00	0.00	0.05
6	6	0.25	-0.14	0.00	-0.23	0.13	0.00	0.00	0.00	0.05
7	1	0.00	0.29	0.00	0.00	0.31	0.00	0.00	0.00	0.57
8	1	-0.25	-0.15	0.00	0.27	0.15	0.00	0.00	0.00	-0.28
9	1	0.25	-0.15	0.00	0.27	-0.15	0.00	0.00	0.00	-0.29
10	1	0.00	0.29	0.00	0.00	-0.31	0.00	0.00	0.00	0.57
11	1	-0.25	-0.15	0.00	-0.27	-0.15	0.00	0.00	0.00	-0.28
12	1	0.25	-0.15	0.00	-0.27	0.15	0.00	0.00	0.00	-0.29

	13	14	15
	E2U	B2G	E1U
Frequencies --	1190.7667	1214.8130	1225.9398
Red. masses --	1.3492	1.2520	1.6196

Frc consts	--	1.1271			1.0886			1.4342			
IR Inten	--	0.0000			0.0000			0.2238			
Raman Activ	--	0.0000			0.0000			0.0000			
Depolar	--	0.0000			0.0000			0.0000			
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	0.00	0.00	0.00	0.00	0.00	-0.06	0.00	0.11	0.00	
2	6	0.00	0.00	-0.09	0.00	0.00	0.06	0.08	-0.03	0.00	
3	6	0.00	0.00	0.09	0.00	0.00	-0.06	-0.08	-0.03	0.00	
4	6	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.11	0.00	
5	6	0.00	0.00	-0.09	0.00	0.00	-0.06	0.08	-0.03	0.00	
6	6	0.00	0.00	0.09	0.00	0.00	0.06	-0.08	-0.03	0.00	
7	1	0.00	0.00	0.00	0.00	0.00	0.40	0.00	0.13	0.00	
8	1	0.00	0.00	0.49	0.00	0.00	-0.40	0.29	-0.38	0.00	
9	1	0.00	0.00	-0.49	0.00	0.00	0.40	-0.29	-0.38	0.00	
10	1	0.00	0.00	0.00	0.00	0.00	-0.40	0.00	0.13	0.00	
11	1	0.00	0.00	0.49	0.00	0.00	0.40	0.29	-0.38	0.00	
12	1	0.00	0.00	-0.49	0.00	0.00	-0.40	-0.29	-0.38	0.00	
		16			17			18			
		E1U			E2G			E2G			
Frequencies	--	1225.9398			1371.4263			1371.4263			
Red. masses	--	1.6196			1.1230			1.1230			
Frc consts	--	1.4342			1.2444			1.2444			
IR Inten	--	0.2238			0.0000			0.0000			
Raman Activ	--	0.0000			12.6519			12.6519			
Depolar	--	0.0000			0.7500			0.7500			
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	-0.08	0.00	0.00	0.00	0.00	0.00	-0.06	0.00	0.00	
2	6	0.06	0.08	0.00	0.03	-0.04	0.00	0.01	-0.03	0.00	
3	6	0.06	-0.08	0.00	0.03	0.04	0.00	-0.01	-0.03	0.00	
4	6	-0.08	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00	
5	6	0.06	0.08	0.00	-0.03	0.04	0.00	-0.01	0.03	0.00	
6	6	0.06	-0.08	0.00	-0.03	-0.04	0.00	0.01	0.03	0.00	
7	1	-0.55	0.00	0.00	0.00	0.00	0.00	-0.57	0.00	0.00	
8	1	-0.04	0.29	0.00	0.25	-0.43	0.00	0.14	-0.25	0.00	
9	1	-0.04	-0.29	0.00	0.25	0.43	0.00	-0.14	-0.25	0.00	
10	1	-0.55	0.00	0.00	0.00	0.00	0.00	0.57	0.00	0.00	
11	1	-0.04	0.29	0.00	-0.25	0.43	0.00	-0.14	0.25	0.00	
12	1	-0.04	-0.29	0.00	-0.25	-0.43	0.00	0.14	0.25	0.00	
		19			20			21			
		B2U			A2G			E1U			
Frequencies	--	1377.1164			1595.3626			1772.6667			
Red. masses	--	1.0769			1.2483			2.1164			
Frc consts	--	1.2033			1.8719			3.9184			
IR Inten	--	0.0000			0.0000			15.1656			
Raman Activ	--	0.0000			0.0000			0.0000			
Depolar	--	0.0000			0.0000			0.0000			
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	-0.03	0.00	0.00	0.06	0.00	0.00	-0.15	0.00	0.00	
2	6	0.02	-0.03	0.00	0.03	-0.05	0.00	0.04	0.11	0.00	
3	6	0.02	0.03	0.00	-0.03	-0.05	0.00	0.04	-0.11	0.00	
4	6	-0.03	0.00	0.00	-0.06	0.00	0.00	-0.15	0.00	0.00	
5	6	0.02	-0.03	0.00	-0.03	0.05	0.00	0.04	0.11	0.00	
6	6	0.02	0.03	0.00	0.03	0.05	0.00	0.04	-0.11	0.00	
7	1	0.41	0.00	0.00	-0.40	0.00	0.00	0.53	0.00	0.00	
8	1	-0.20	0.35	0.00	-0.20	0.35	0.00	0.23	-0.18	0.00	
9	1	-0.20	-0.35	0.00	0.20	0.35	0.00	0.23	0.18	0.00	
10	1	0.41	0.00	0.00	0.40	0.00	0.00	0.53	0.00	0.00	
11	1	-0.20	0.35	0.00	0.20	-0.35	0.00	0.23	-0.18	0.00	

12	1	-0.20	-0.35	0.00	-0.20	-0.35	0.00	0.23	0.18	0.00	
			22			23			24		
			E1U			E2G			E2G		
Frequencies --			1772.6667			1932.5853			1932.5853		
Red. masses --			2.1164			5.5111			5.5111		
Frc consts --			3.9184			12.1274			12.1274		
IR Inten --			15.1656			0.0000			0.0000		
Raman Activ --			0.0000			21.6341			21.6341		
Depolar --			0.0000			0.7500			0.7500		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	0.00	-0.10	0.00	0.00	0.15	0.00	-0.34	0.00	0.00	
2	6	-0.11	0.09	0.00	0.08	-0.29	0.00	0.19	-0.08	0.00	
3	6	0.11	0.09	0.00	0.08	0.29	0.00	-0.19	-0.08	0.00	
4	6	0.00	-0.10	0.00	0.00	-0.15	0.00	0.34	0.00	0.00	
5	6	-0.11	0.09	0.00	-0.08	0.29	0.00	-0.19	0.08	0.00	
6	6	0.11	0.09	0.00	-0.08	-0.29	0.00	0.19	0.08	0.00	
7	1	0.00	-0.13	0.00	0.00	0.19	0.00	0.40	0.00	0.00	
8	1	0.18	-0.43	0.00	-0.26	0.25	0.00	0.04	0.26	0.00	
9	1	-0.18	-0.43	0.00	-0.26	-0.25	0.00	-0.04	0.26	0.00	
10	1	0.00	-0.13	0.00	0.00	-0.19	0.00	-0.40	0.00	0.00	
11	1	0.18	-0.43	0.00	0.26	-0.25	0.00	-0.04	-0.26	0.00	
12	1	-0.18	-0.43	0.00	0.26	0.25	0.00	0.04	-0.26	0.00	
			25			26			27		
			B1U			E2G			E2G		
Frequencies --			3704.2088			3722.6353			3722.6354		
Red. masses --			1.0878			1.0936			1.0936		
Frc consts --			8.7939			8.9295			8.9295		
IR Inten --			0.0000			0.0000			0.0000		
Raman Activ --			0.0000			75.9104			75.9104		
Depolar --			0.0000			0.7500			0.7500		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	0.00	-0.03	0.00	0.00	0.05	0.00	0.00	0.00	0.00	
2	6	0.03	0.02	0.00	-0.02	-0.02	0.00	-0.04	-0.02	0.00	
3	6	-0.03	0.02	0.00	-0.02	0.02	0.00	0.04	-0.02	0.00	
4	6	0.00	-0.03	0.00	0.00	-0.05	0.00	0.00	0.00	0.00	
5	6	0.03	0.02	0.00	0.02	0.02	0.00	0.04	0.02	0.00	
6	6	-0.03	0.02	0.00	0.02	-0.02	0.00	-0.04	0.02	0.00	
7	1	0.00	0.41	0.00	0.00	-0.58	0.00	0.00	0.00	0.00	
8	1	-0.35	-0.20	0.00	0.25	0.15	0.00	0.43	0.25	0.00	
9	1	0.35	-0.20	0.00	0.25	-0.15	0.00	-0.43	0.25	0.00	
10	1	0.00	0.41	0.00	0.00	0.58	0.00	0.00	0.00	0.00	
11	1	-0.35	-0.20	0.00	-0.25	-0.15	0.00	-0.43	-0.25	0.00	
12	1	0.35	-0.20	0.00	-0.25	0.15	0.00	0.43	-0.25	0.00	
			28			29			30		
			E1U			E1U			A1G		
Frequencies --			3736.3254			3736.3255			3747.1796		
Red. masses --			1.1020			1.1020			1.1069		
Frc consts --			9.0638			9.0638			9.1574		
IR Inten --			8.8014			8.8014			0.0000		
Raman Activ --			0.0000			0.0000			192.0229		
Depolar --			0.0000			0.0000			0.1174		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	0.00	-0.05	0.00	-0.01	0.00	0.00	0.00	0.04	0.00	
2	6	-0.03	-0.01	0.00	0.04	0.03	0.00	0.03	0.02	0.00	
3	6	0.03	-0.01	0.00	0.04	-0.03	0.00	0.03	-0.02	0.00	
4	6	0.00	-0.05	0.00	-0.01	0.00	0.00	0.00	-0.04	0.00	
5	6	-0.03	-0.01	0.00	0.04	0.03	0.00	-0.03	-0.02	0.00	
6	6	0.03	-0.01	0.00	0.04	-0.03	0.00	-0.03	0.02	0.00	

```
  7   1     0.00   0.57   0.00     0.00   0.00   0.00     0.00  -0.41   0.00
  8   1     0.25   0.14   0.00    -0.43  -0.25   0.00    -0.35  -0.20   0.00
  9   1    -0.25   0.14   0.00    -0.43   0.25   0.00    -0.35   0.20   0.00
 10   1     0.00   0.57   0.00     0.00   0.00   0.00     0.00   0.41   0.00
 11   1     0.25   0.14   0.00    -0.43  -0.25   0.00     0.35   0.20   0.00
 12   1    -0.25   0.14   0.00    -0.43   0.25   0.00     0.35  -0.20   0.00
-------------------
- THERMOCHEMISTRY -
-------------------
TEMPERATURE   298.150 KELVIN.
PRESSURE      1.00000 ATM.
ATOM  1 HAS ATOMIC NUMBER  6 AND MASS  12.00000
ATOM  2 HAS ATOMIC NUMBER  6 AND MASS  12.00000
ATOM  3 HAS ATOMIC NUMBER  6 AND MASS  12.00000
ATOM  4 HAS ATOMIC NUMBER  6 AND MASS  12.00000
ATOM  5 HAS ATOMIC NUMBER  6 AND MASS  12.00000
ATOM  6 HAS ATOMIC NUMBER  6 AND MASS  12.00000
ATOM  7 HAS ATOMIC NUMBER  1 AND MASS   1.00783
ATOM  8 HAS ATOMIC NUMBER  1 AND MASS   1.00783
ATOM  9 HAS ATOMIC NUMBER  1 AND MASS   1.00783
ATOM 10 HAS ATOMIC NUMBER  1 AND MASS   1.00783
ATOM 11 HAS ATOMIC NUMBER  1 AND MASS   1.00783
ATOM 12 HAS ATOMIC NUMBER  1 AND MASS   1.00783
Molecular mass:    78.04695 amu.
Principle axes and moments of inertia in atomic units:
                         1         2         3
    EIGENVALUES --   313.07268 313.07268 626.14536
          X            0.90668  -0.42182   0.00000
          Y            0.42182   0.90668   0.00000
          Z            0.00000   0.00000   1.00000
THIS MOLECULE IS AN OBLATE SYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER 12.
ROTATIONAL TEMPERATURES (KELVIN)      0.27666     0.27666     0.13833
ROTATIONAL CONSTANTS (GHZ)            5.76461     5.76461     2.88230
ZERO-POINT VIBRATIONAL ENERGY     305717.3 (JOULES/MOL)
                                  73.06819 (KCAL/MOL)
                                 0.1164416 (HARTREE/PARTICLE)
WARNING-- EXPLICIT CONSIDERATION OF   2 DEGREES OF FREEDOM AS
          VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
VIBRATIONAL TEMPERATURES:    687.80   687.80  1007.40  1007.40  1167.21
         (KELVIN)           1210.30  1493.36  1493.36  1661.08  1664.27
                            1686.97  1713.24  1713.24  1747.83  1763.84
                            1763.84  1973.17  1973.17  1981.35  2295.36
                            2550.46  2550.46  2780.54  2780.54  5329.50
                            5356.01  5356.01  5375.71  5375.71  5391.32
SUM OF THERMAL ENERGIES:    0.1203595 (HARTREE/PARTICLE)
SUM OF HARTREE-FOCK AND THERMAL ENERGIES: -227.7710009 (HARTREE/PARTICLE)
                        E                 CV                S
                   JOULES/MOL     JOULES/MOL-KELVIN   JOULES/MOL-KELVIN
TOTAL              316003.883            59.776            262.184
ELECTRONIC              0.000             0.000              0.000
TRANSLATIONAL        3718.457            12.472            163.090
ROTATIONAL           3718.457            12.472             86.537
VIBRATIONAL        308566.968            34.832             12.558
VIBRATION  1         3491.750             5.434              2.993
VIBRATION  2         3491.750             5.434              2.993
                        E                 CV                S
                    KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
```

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TOTAL                    75.527             14.287             62.664
ELECTRONIC                0.000              0.000              0.000
TRANSLATIONAL             0.889              2.981             38.979
ROTATIONAL                0.889              2.981             20.683
VIBRATIONAL              73.749              8.325              3.001
VIBRATION  1              0.835              1.299              0.715
VIBRATION  2              0.835              1.299              0.715
                     Q            LOG10(Q)             LN(Q)
TOTAL BOT       0.000000E+00        -42.100701        -97.301252
TOTAL V=0       0.287304E+12         11.458341         26.023000
VIB (BOT)       0.000000E+00        -53.402346       -122.963447
VIB (BOT)  1    0.350438E+00         -0.455388         -1.048570
VIB (BOT)  2    0.350438E+00         -0.455388         -1.048570
VIB (V=0)       0.143448E+01          0.156696          0.360806
VIB (V=0)  1    0.111058E+01          0.045550          0.104882
VIB (V=0)  2    0.111058E+01          0.045550          0.104882
ELECTRONIC      0.100000E+01          0.000000          0.000000
TRANSLATIONAL   0.271016E+08          7.432994         17.115102
ROTATIONAL      0.739011E+04          3.868651          8.907898
        Item               Value     Threshold  Converged?
Maximum Force            0.000208     0.000450     YES
RMS     Force            0.000173     0.000300     YES
Maximum Displacement     0.000050     0.001800     YES
RMS     Displacement     0.000047     0.001200     YES
Predicted change in energy=-8.007852D-09
Optimization completed.
   -- Stationary point found.
                     ----------------------------
                     !  Optimized Parameters   !
                     ! (Angstroms and Degrees) !
---------------------                          ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------------
!       CX          1.3868   -DE/DX =    0.000208                     !
!       CH          1.0826   -DE/DX =   -0.000129                     !
--------------------------------------------------------------------------------
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

ORBITAL SYMMETRIES.
      OCCUPIED  (E1U) (E1U) (A1G) (E2G) (E2G) (B1U) (A1G) (E1U)
                (E1U) (E2G) (E2G) (A1G) (B1U) (B2U) (E1U) (E1U)
                (A2U) (E2G) (E2G) (E1G) (E1G)
      VIRTUAL   (E2U) (E2U) (B2G) (A1G) (E1U) (E1U) (B1U) (E2G)
                (E2G) (E2G) (E2G) (E1U) (E1U) (A2G) (B1U)
 THE ELECTRONIC STATE IS 1-A1G.
Alpha eigenvalues --  -11.02925 -11.02925 -11.02924 -11.02885 -11.02885
Alpha eigenvalues --  -11.02868  -1.09568  -0.95814  -0.95814  -0.76899
Alpha eigenvalues --   -0.76899  -0.66572  -0.59364  -0.55728  -0.53608
Alpha eigenvalues --   -0.53608  -0.46092  -0.43377  -0.43377  -0.28266
Alpha eigenvalues --   -0.28266   0.27077   0.27077   0.50913   0.57914
Alpha eigenvalues --    0.64986   0.64986   0.72909   0.74359   0.74359
Alpha eigenvalues --    0.89014   0.89014   0.90631   0.90631   1.09947
Alpha eigenvalues --    1.16393
Total atomic charges:
             1
 1  C   -0.062919
 2  C   -0.062919
 3  C   -0.062919
```

```
 4  C   -0.062919
 5  C   -0.062919
 6  C   -0.062919
 7  H    0.062919
 8  H    0.062919
 9  H    0.062919
10  H    0.062919
11  H    0.062919
12  H    0.062919
Sum of Mulliken charges=   0.00000
Charge= 0.0000 esu
Dipole moment (Debye):
   X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=     0.0000
Quadrupole moment (Debye-Ang):
  XX=   -31.2299   YY=   -31.2299   ZZ=   -35.0716
  XY=     0.0000   XZ=     0.0000   YZ=     0.0000
Octapole moment (Debye-Ang**2):
 XXX=     0.0000  YYY=     0.0000  ZZZ=     0.0000  XYY=     0.0000
 XXY=     0.0000  XXZ=     0.0000  XZZ=     0.0000  YZZ=     0.0000
 YYZ=     0.0000  XYZ=     0.0000
Hexadecapole moment (Debye-Ang**3):
XXXX=  -258.0210 YYYY=  -258.0210 ZZZZ=   -28.4756 XXXY=     0.0000
XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=     0.0000
ZZZY=     0.0000 XXYY=   -86.0070 XXZZ=   -53.2449 YYZZ=   -53.2449
XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
N-N= 2.045361003939D+02 E-N=-9.399037518418D+02  KE= 2.260621385293D+02
 Exact polarizability:  45.193   0.000  45.193   0.000   0.000   5.855
Approx polarizability:  45.423   0.000  45.423   0.000   0.000   4.900
Unable to assign archive entry number now.

ART, GLORY, FREEDOM FAIL, BUT NATURE STILL IS FAIR.

                                          -- BYRON

Final File Lengths (Blocks):
GAUSS_RWF      13824 -- deleted
GAUSS_INT       2541 -- deleted
GAUSS_CHK       1041

Time used:
 IO time  0 days  0 hours  7 minutes 34.3 seconds.
CPU time  0 days  1 hours 32 minutes  4.4 seconds.
TOT time  0 days  1 hours 39 minutes 38.7 seconds.
  RAINER       job terminated at 26-SEP-1993 19:29:35.50

  Accounting information:
  Buffered I/O count:         2378      Peak working set size: 10200
  Direct I/O count:          22716      Peak page file size:   25266
  Page faults:               56731      Mounted volumes:           0
  Charged CPU time:     0 01:32:05.32   Elapsed time:     0 02:20:17.05
```