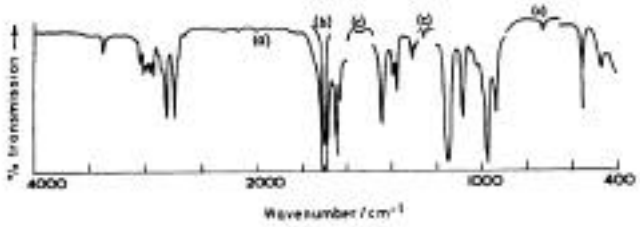
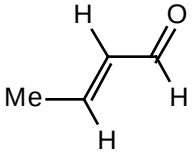
Chemistry 416 "Spectroscopy"
Winter Semester 1996
Dr. Rainer Glaser

Second 1-Hour Examination
"IR/Raman Spectroscopy"

Wednesday, March 6, 1996, 8:40 - 9:30





?

Name:

Question 1	10	
Question 2	10	
Question 3	18	
Question 4	12	
Question 5	10	
Question 6	40	
Total	100	

Vibrational Properties of Crotonaldehyde.

Feel free to use any book and even your notes during this test. In addition, this test comes with the following pieces of supplemental material.

(1) The IR and Raman spectra of crotonaldehyde are taken from the book *Modern Spectroscopy*, 2nd edition, by J. Michael Hollas (published by John Wiley and Sons, **1992**, see pages 150ff). References to the original literature can be found there.

(2) The frequencies and descriptions of the normal modes are listed in Table 6.4 which has been reproduced from Hollas' book.

(3) Also attached are the outputs of <u>two</u> *ab initio* calculations of two different conformations of crotonaldehyde.

Question 1. Composition of the IR Spectrum. (10 points)

As you can see from the figure legend, the IR vibrational spectrum shown in Figure 6.15 is a composite of three spectra. Explain why one might want to record some parts "(a)" of the spectrum in 10% CCl_4 while another section "(b)" is recorded in 1% CCl_4 solution. Then explain why section "(c)" was recorded using a thin film.

Why 10% or 1% CCl_4 solution? (5 points)
Why a thin film? (5 points)

Question 2. Sample Preparation. (10 points)

Describe (use schematic drawings as necessary, specify window materials and so on) how the samples have to be prepared for the recording of ...

... the solution IR spectra (3 points):
... the thin film IR spectrum (3 points):
... the Raman spectrum of the neat liquid (4 points):

Question 3. Characteristic Bands. (18 points)

(a) Using the spectra and the table provided, identify the bands associated with the C=O stretching and with the C=C stretching vibrations. (Just find the numbers and write them down in the spaces below.)

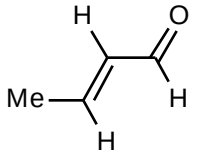
	IR	RAMAN
C=O stretch		
C=C stretch		

(b) Note that the IR and Raman frequencies for the CO stretch differ. How come? (4 points)

(c) Suppose you would want to make sure that the band assigned to the CO stretching vibration is correct. How could you ascertain the assignment using a heavier isotope of oxygen? Specify what isotope you would use and what consequences that would have on the spectrum. State effects on force constant k and reduced mass μ, provide equation for $\nu = f(k, \mu)$. (10 points)

Question 4. Prediction of the Spectrum of Crotonaldehyde. (12 points)

Using the book by Pretsch et al. or any other similar book, predict the frequencies for the two most characteristic stretching vibrations, the CO stretch and the CC stretch. Also provide estimates for the CO in CH_3CHO and the C=C in 2-butene. Provide the predicetd value and write down precisely where you found it (book and page number).



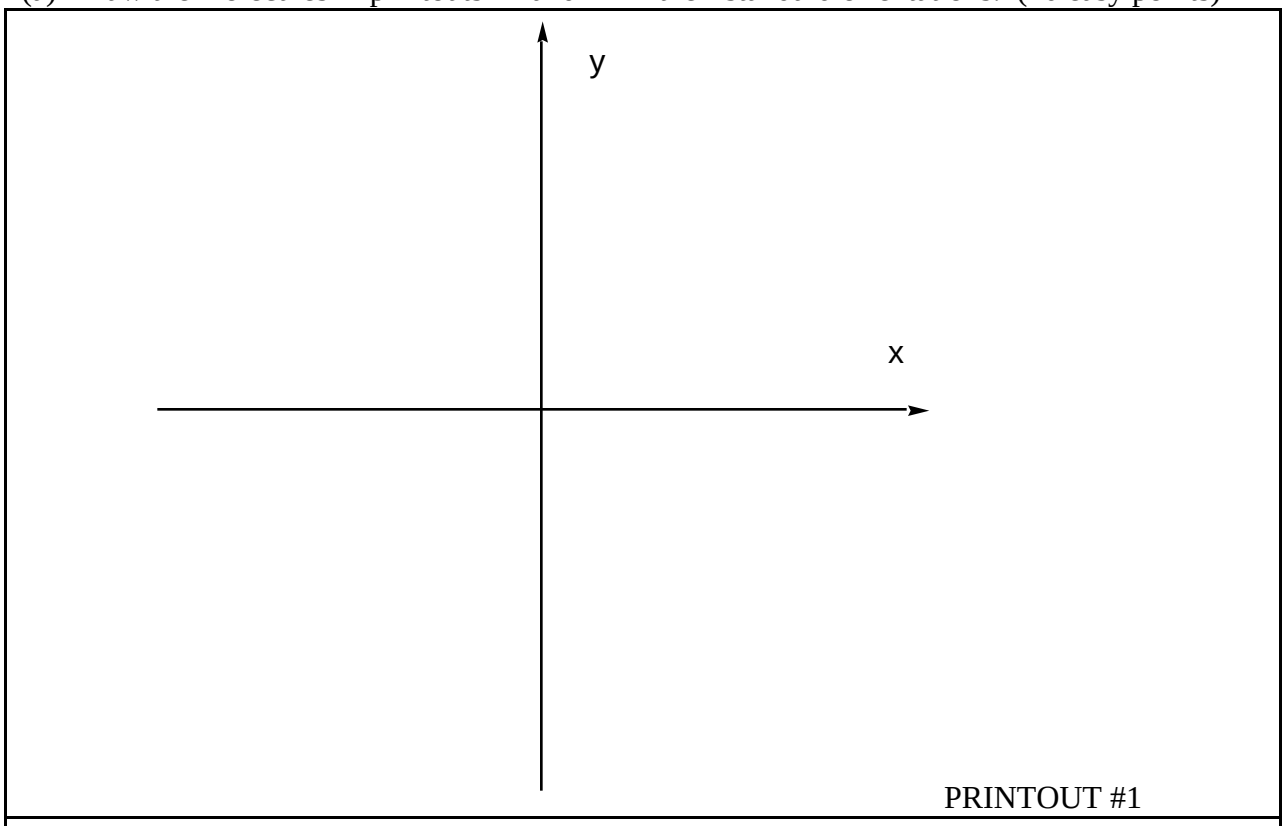
CO in acetaldehyde:	C=C in 2-Butene (-HC=CH-):
Predict C=O in CA:	Predict C=C in CA:

Question 5. The strong bands in the 2950-2700 cm^{-1} region. (10 points).

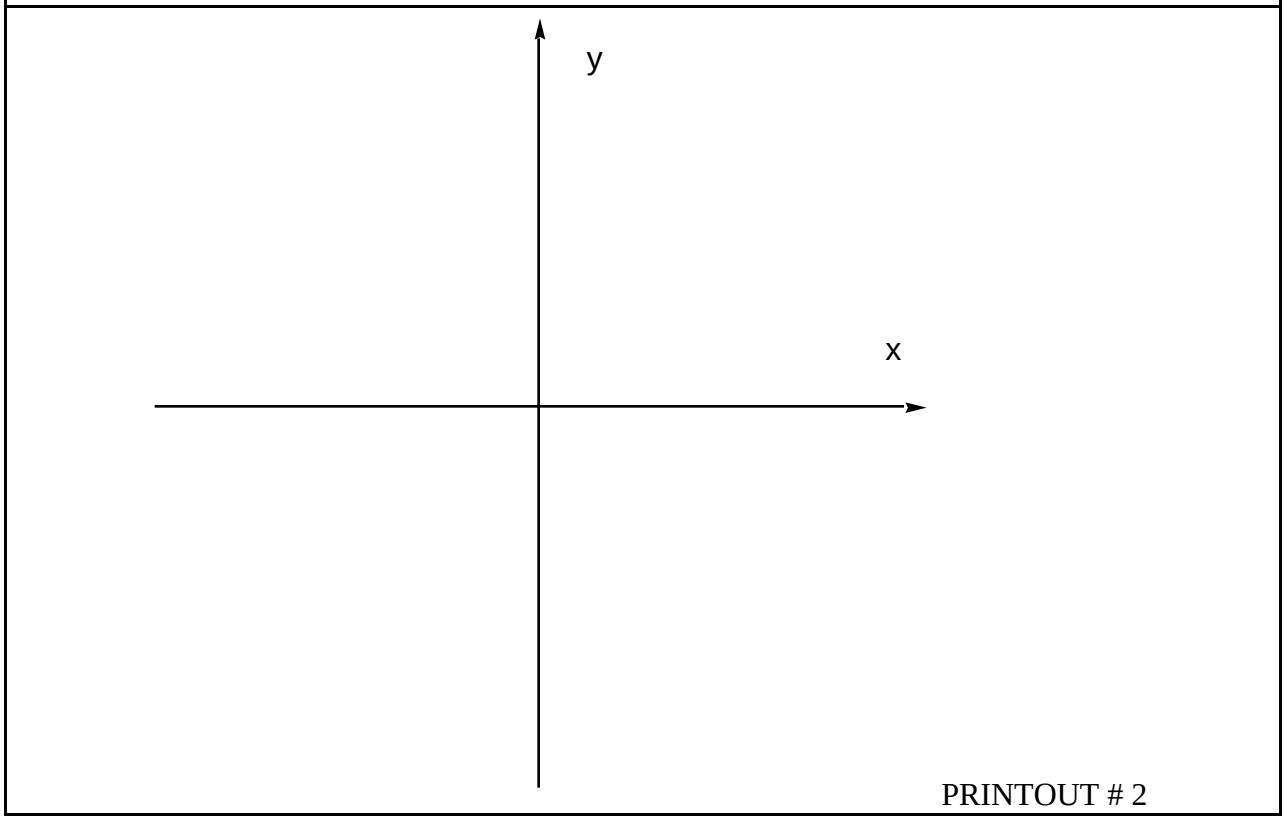
Explain the term "Fermi doublet". Fermi doublets are quite frequent in aldehydes. Explain what modes interact in the case of aldehydes to produce the Fermi doublet.

Question 6. Normal Modes. (40 points)

(a) Draw the molecules in printouts #1 and #2 in their standard orientations. (10 easy points)

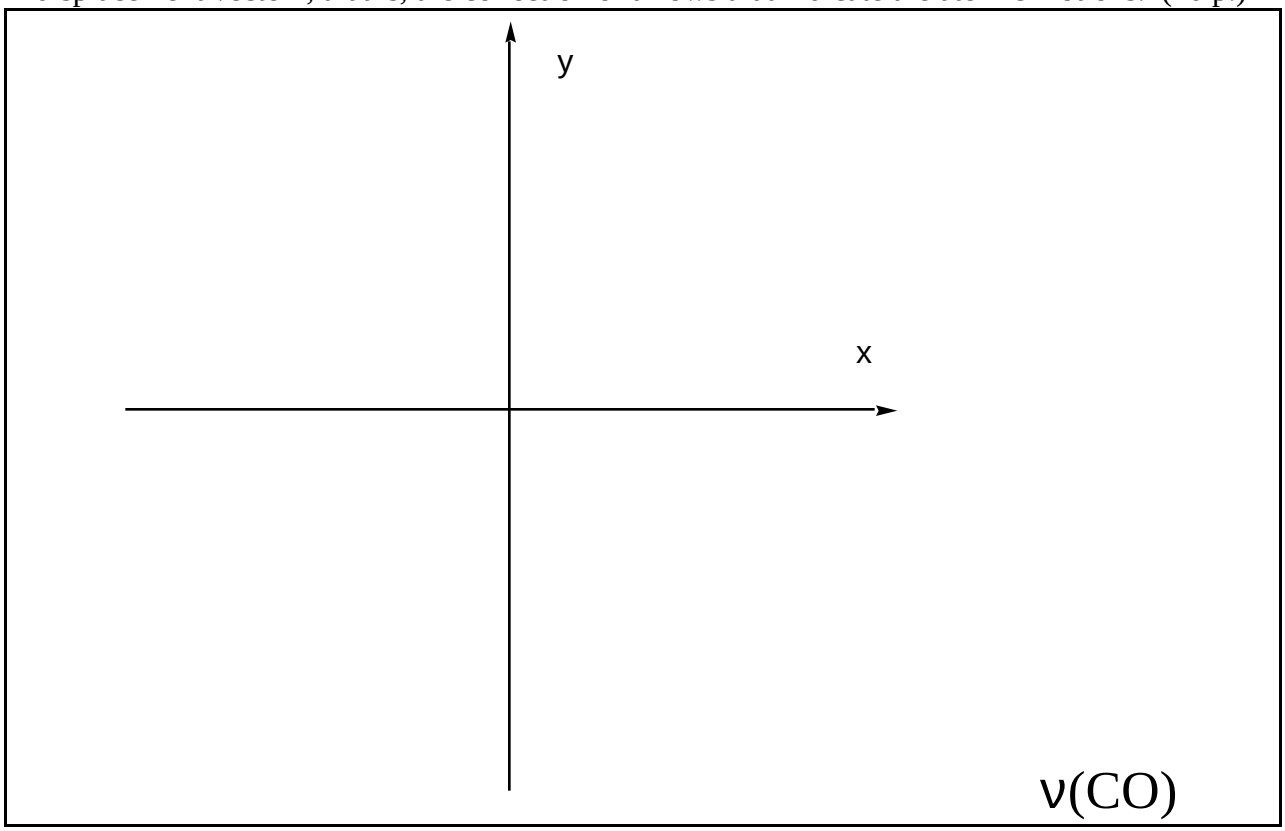


PRINTOUT #1



PRINTOUT # 2

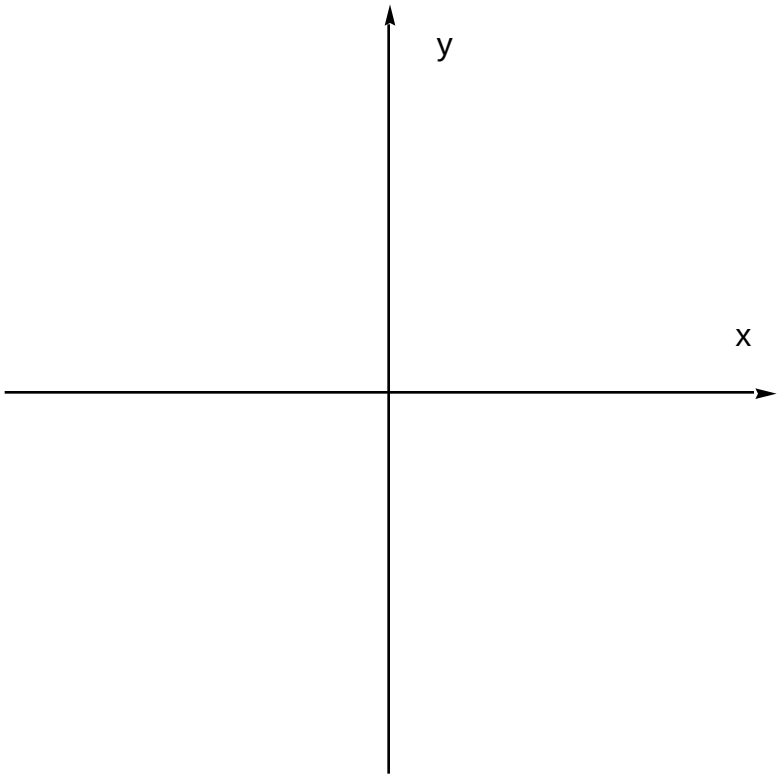
(b) In printout #1, find the normal mode that corresponds to the CO stretch and draw the "displacement vector", that is, the collection of arrows that indicate the atomic motions. (10 p.)



(c) The frequency calculated for the CO stretching mode is _____ cm^{-1}. At this level of theory, the vibrational frequencies usually are overestimated rather consistently by about 10 percent. Taking this into account, theory would predict a frequency of _____ cm^{-1} for this mode which is still some _____ cm^{-1} too high. The case of this CO stretch is extreme and theory is able to predict frequencies generally much better. The great deviation for CO stretch is due to the high polarity of the CO bond. To get bonds like that right one needs to use higher level theory that account for electron correlation. (6 points).

(d) The CO stretch is *by far* the strongest band in the IR spectrum (while it is not the strongest band in the Raman spectrum). Briefly explain why the IR intensity of ν(CO) is so high. (4 p.)

(e) In printout #2, the lowest vibrational frequency is in fact negative! This is a so-called "imaginary" vibration. Whenever one imaginary mode occurs, then the structure is a transition state and the displacement vector associated with that imaginary vibration tells you what is in transition. Draw the "displacement vector" of the imaginary mode of printout #2 and state what transition state we are looking at. (10 points)



ν=-203 cm^{-1}

Considering the imaginary normal mode, the structure computed in #2 is the transitioon state structure for .....

The End of another Exciting Learning Experience. Relax.

Supplemental Material

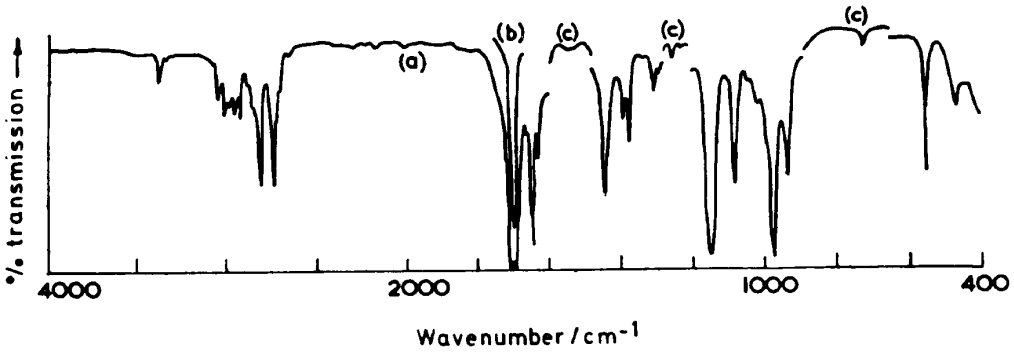


Figure 6.15 The infrared vibrational spectrum of crotonaldehyde. The parts marked (a), (b), and (c) refer to a 10 per cent (by volume) solution in CCl_4, a 1 per cent solution in CCl_4, and a thin liquid film respectively. (Reproduced, with permission, from Bowles, A. J., George, W. O., and Maddams, W. F., *J. Chem. Soc.* (*B*), 810, 1969.)

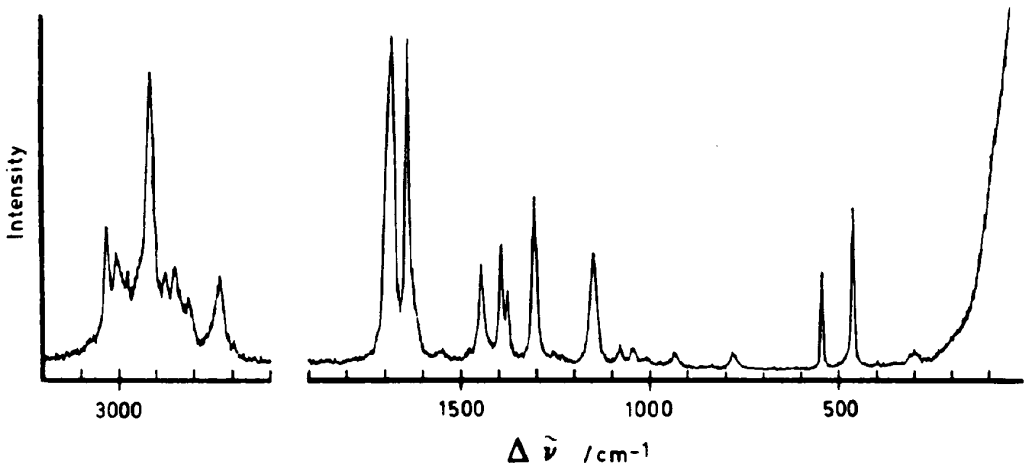


Figure 6.17 The laser Raman vibrational spectrum of liquid crotonaldehyde. (Reproduced, with permission, from Durig, J. R., Brown, S. C., Kalasinsky, V. F., and George, W. O., *Spectrochim. Acta*, **32A**, 807, 1976. Copyright (1976) Pergamon Press.)

Table 6.4 Fundamental vibration wavenumbers of crotonaldehyde obtained from the infra-red and Raman spectra.

Vib.	Approximate description	IR exp.	RAMAN exp.
	in plane		
1	CH antisym. stretch on C=C	3042	3032
2	CH symmetric stretch on C=C	3002	3006
3	CH, antisymmetric stretch	2944	2949
4	CH_3 symmetric stretch	2916	2918
5	CH stretch on CHO	2727	2732
6	C=O stretch	1693	1682
7	C=C stretch	1641	1641
8	CH_3 antisym. deformation	1444	1445
9	CH rock (in-pl. bend) on CHO	1389	1393
10	CH, sym. deformation	1375	t380
11	CH sym. deform. on C=C	1305	1306
12	CH antisym. def. on C=C	1253	1252
13	CH_3in-plane rock	1075	1080
14	C-CHO stretch	1042	1046
15	C-CH_3 stretch	931	931
16	CH_3-C=C bend	542	545
17	C=C-C bend	459	464
18	C-C=O bend	216	230
	out-of-plane		
19	CH, antisym. stretch	2982	2976
20	CH, antisym. deformation	1444	1445
21	CH_3 rock	1146	1149
22	CH antisym. deformation on C=C	966	
23	CH sym. deformation on C=C		780
24	CH wag (o-o-p bend) on CHO	727	
25	CH_3 bend	297	300
26	CH_3 torsion	173	
27	CHO torsion	121	

PRINTOUT #1

```
*****************************************************
 Gaussian 92:  IBM-RS6000-G92/DFT-RevG.4  7-Sep-1994
                    4-Mar-1996
 *****************************************************
 %chk=croton2
 Default route: MaxDisk=240000000 SCF=Direct
 ----------------------------------------------
 # rhf/6-31G* freq guess=read geom=checkpoint
 ----------------------------------------------
 1/10=4,29=10002,30=1/1,3;
 2/12=2,17=6,18=5/2;
 3/5=1,6=6,7=1,11=1,25=1,30=1/1,2,3;
 4/5=1,7=1/1;
 5/5=2/2;
 8/6=4,11=11,27=240000000/1;
 10/13=10/2;
 11/6=2,8=1,9=11,15=111,16=11/1,2,10;
 10/6=1,9=1/2;
 7/8=1,10=1,25=1/1,2,3,16;
 1/10=4,30=1/3;
 6/7=2,8=2,9=2,10=2,18=1,28=1/1;
 99//99;
 ------------------------------------------------------
 Crotonaldehyde, eclipsed, Cs, rhf/6-31G* -- Frequencies
 ------------------------------------------------------
 Z-Matrix taken from the checkpoint file:
 croton2.chk
    Charge = 0 Multiplicity = 1
 C
 O,1,co
 H,1,hc1,2,hco
 C,1,cc1,2,cco,3,180.,0
 H,4,hca,1,hcca,2,0.,0
 C,4,cc2,1,ccc1,2,180.,0
 H,6,hc3,4,hccb,1,0.,0
 C,6,cc3,4,ccc2,1,180.,0
 H,8,hcip,7,hcipang,4,0.,0
 H,8,hcoop,7,hcoopang,4,di,0
 H,8,hcoop,7,hcoopang,4,-di,0
      Variables:
 co=1.19092879
 hc1=1.09552275
 cc1=1.47377814
 hca=1.07629926
 cc2=1.32404928
 hc3=1.07987394
 cc3=1.49844724
 hcip=1.08315813
 hcoop=1.08645033
 hco=120.62132958
 cco=124.1074518
 hcca=116.47237407
 ccc1=121.23244057
```

```
hccb=118.50084663
ccc2=125.63319984
hcipang=137.8909386
hcoopang=95.83313148
di=126.07132418
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                      ---------------------------
                      !   Initial Parameters    !
                      ! (Angstroms and Degrees) !
---------------------                           ----------------------
!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------------
!       co          1.1909   calculate D2E/DX2 analytically            !
!       hc1         1.0955   calculate D2E/DX2 analytically            !
!       cc1         1.4738   calculate D2E/DX2 analytically            !
!       hca         1.0763   calculate D2E/DX2 analytically            !
!       cc2         1.324    calculate D2E/DX2 analytically            !
!       hc3         1.0799   calculate D2E/DX2 analytically            !
!       cc3         1.4984   calculate D2E/DX2 analytically            !
!      hcip         1.0832   calculate D2E/DX2 analytically            !
!      hcoop        1.0865   calculate D2E/DX2 analytically            !
!       hco       120.6213   calculate D2E/DX2 analytically            !
!       cco       124.1075   calculate D2E/DX2 analytically            !
!      hcca       116.4724   calculate D2E/DX2 analytically            !
!      ccc1       121.2324   calculate D2E/DX2 analytically            !
!      hccb       118.5008   calculate D2E/DX2 analytically            !
!      ccc2       125.6332   calculate D2E/DX2 analytically            !
!     hcipang     137.8909   calculate D2E/DX2 analytically            !
!    hcoopang      95.8331   calculate D2E/DX2 analytically            !
!       di        126.0713   calculate D2E/DX2 analytically            !
--------------------------------------------------------------------------------
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  28 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
--------------------------------------------------------------------------------
                      Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
--------------------------------------------------------------------------------
  1   1  C
  2   2  O     1   1.190929(  1)
  3   3  H     1   1.095523(  2)   2  120.621( 11)
  4   4  C     1   1.473778(  3)   2  124.107( 12)   3  180.000( 20)   0
  5   5  H     4   1.076299(  4)   1  116.472( 13)   2     .000( 21)   0
  6   6  C     4   1.324049(  5)   1  121.232( 14)   2  180.000( 22)   0
  7   7  H     6   1.079874(  6)   4  118.501( 15)   1     .000( 23)   0
  8   8  C     6   1.498447(  7)   4  125.633( 16)   1  180.000( 24)   0
  9   9  H     8   1.083158(  8)   7  137.891( 17)   4     .000( 25)   0
 10  10  H     8   1.086450(  9)   7   95.833( 18)   4  126.071( 26)   0
 11  11  H     8   1.086450( 10)   7   95.833( 19)   4 -126.071( 27)   0
--------------------------------------------------------------------------------
                Z-Matrix orientation:
---------------------------------------------------------
```

```
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------
   1          6            .000000     .000000     .000000
   2          8            .000000     .000000    1.190929
   3          1            .942755     .000000    -.558017
   4          6          -1.220270     .000000    -.826416
   5          1          -2.157770     .000000    -.297727
   6          6          -1.153859     .000000   -2.148799
   7          1           -.180204     .000000   -2.615836
   8          6          -2.326422     .000000   -3.081772
   9          1          -3.265781     .000000   -2.542480
  10          1          -2.299315     .873614   -3.727092
  11          1          -2.299315    -.873614   -3.727092
---------------------------------------------------------------
                  Distance matrix (angstroms):
             1          2          3          4          5
 1  C     .000000
 2  O    1.190929    .000000
 3  H    1.095523   1.986857    .000000
 4  C    1.473778   2.357698   2.179613    .000000
 5  H    2.178214   2.621463   3.111432   1.076299    .000000
 6  C    2.439001   3.533436   2.631801   1.324049   2.105779
 7  H    2.622036   3.811028   2.344281   2.069725   3.047031
 8  C    3.861290   4.864999   4.129995   2.512012   2.789149
 9  H    4.138784   4.960208   4.652942   2.670017   2.503319
10  H    4.465565   5.498817   4.617061   3.215815   3.541721
11  H    4.465565   5.498817   4.617061   3.215815   3.541721
             6          7          8          9         10
 6  C     .000000
 7  H    1.079874    .000000
 8  C    1.498447   2.196213    .000000
 9  H    2.148302   3.086449   1.083158    .000000
10  H    2.136886   2.547298   1.086450   1.760842    .000000
11  H    2.136886   2.547298   1.086450   1.760842   1.747228
            11
11  H     .000000
                        Interatomic angles:
      O2-C1-H3=120.6213       O2-C1-C4=124.1075       H3-C1-C4=115.2712
      C1-C4-H5=116.4724       C1-C4-C6=121.2324       H5-C4-C6=122.2952
      C4-C6-H7=118.5008       C4-C6-C8=125.6332       H7-C6-C8=115.866
      C6-C8-H9=111.6314      C6-C8-H10=110.5056      H9-C8-H10=108.5039
     C6-C8-H11=110.5056      H9-C8-H11=108.5039     H10-C8-H11=107.0467
STOICHIOMETRY    C4H6O
FRAMEWORK GROUP  CS[SG(C4H4O),X(H2)]
DEG. OF FREEDOM   18
FULL POINT GROUP                 CS      NOP  2
LARGEST ABELIAN SUBGROUP         CS      NOP  2
LARGEST CONCISE ABELIAN SUBGROUP CS      NOP  2
                 Standard orientation:
---------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------
```

```
   1          6          -1.446779     .050162     .000000
   2          8          -2.290236     .890931     .000000
   3          1          -1.717135   -1.011477     .000000
   4          6            .000000     .330968     .000000
   5          1            .287418    1.368181     .000000
   6          6            .889673    -.649639     .000000
   7          1            .533066   -1.668932     .000000
   8          6           2.378240    -.477847     .000000
   9          1           2.659460     .568168     .000000
  10          1           2.816141    -.952626     .873614
  11          1           2.816141    -.952626    -.873614
---------------------------------------------------------
Rotational constants (GHZ):     33.4328901      2.2005535      2.0909396
Isotopes: C-12,O-16,H-1,C-12,H-1,C-12,H-1,C-12,H-1,H-1,H-1
Standard basis: 6-31G(D)     (S, S=P, 6D, 7F)
There are    65 symmetry adapted basis functions of A'  symmetry.
There are    22 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.829.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   87 basis functions      164 primitive gaussians
   19 alpha electrons       19 beta electrons
      nuclear repulsion energy       154.1238778911 Hartrees.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
The smallest eigenvalue of the overlap matrix is  3.011D-03
DipDrv:  MaxL=4.
DipDrv:  will hold 34 matrices at once.
Initial guess read from the checkpoint file:
croton2.chk
Guess basis functions will be translated to current atomic coordinates.
INITIAL GUESS ORBITAL SYMMETRIES.
      OCCUPIED  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A") (A') (A") (A') (A') (A")
      VIRTUAL   (A") (A') (A') (A") (A') (A") (A') (A') (A') (A')
                (A') (A') (A') (A") (A") (A') (A') (A") (A') (A")
                (A') (A') (A') (A') (A') (A') (A") (A') (A') (A')
                (A') (A") (A') (A') (A') (A') (A") (A') (A") (A")
                (A') (A") (A') (A') (A') (A") (A') (A") (A') (A')
                (A') (A") (A') (A") (A') (A') (A") (A') (A") (A')
                (A') (A') (A') (A') (A') (A') (A') (A')
Alpha deviation from unit magnitude is 1.62D-14 for orbital   57.
Alpha deviation from orthogonality  is 1.24D-14 for orbitals  57  31.
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) =  -229.803973415     A.U. after    1 cycles
            Convg  =     .7046D-09             -V/T =  2.0013
            S**2   =    .0000
Range of M.O.s used for correlation:     1    87
Full mass-weighted force constant matrix:
Low frequencies ---   -3.6777    -.7525    -.0029    -.0019     .0020    8.0290
Low frequencies ---  136.4098  209.6515  226.0603
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:

***** edited for brevity ******

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		
		A"			A"			A'		
Frequencies --		136.4097			209.6514			226.0602		
Red. masses --		2.5634			1.3433			3.5167		
Frc consts --		.0281			.0348			.1059		
IR Inten --		3.8229			.3383			9.0271		
Raman Activ --		.0790			2.6359			.0296		
Depolar --		.7500			.7500			.1734		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	.00	.12	.00	.00	.01	-.09	-.05	.00
2	8	.00	.00	-.21	.00	.00	-.05	.13	.18	.00
3	1	.00	.00	.30	.00	.00	-.10	-.34	.02	.00
4	6	.00	.00	.22	.00	.00	.15	-.06	-.26	.00
5	1	.00	.00	.29	.00	.00	.33	-.05	-.26	.00
6	6	.00	.00	.06	.00	.00	-.05	.02	-.18	.00
7	1	.00	.00	-.03	.00	.00	-.22	.20	-.25	.00
8	6	.00	.00	-.13	.00	.00	-.04	-.02	.21	.00
9	1	.00	.00	.24	.00	.00	-.54	-.35	.30	.00
10	1	.17	-.36	-.41	-.07	.44	.24	.13	.36	.00
11	1	-.17	.36	-.41	.07	-.44	.24	.13	.36	.00

		4			5			6		
		A"			A'			A'		
Frequencies --		307.6051			491.8278			583.7872		
Red. masses --		2.1876			3.4959			4.2020		
Frc consts --		.1220			.4982			.8437		
IR Inten --		9.9595			2.2072			14.7101		
Raman Activ --		.6841			5.1081			2.5264		
Depolar --		.7500			.2284			.3815		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	.00	-.19	.22	.02	.00	.00	-.26	.00
2	8	.00	.00	.05	.12	-.09	.00	.31	.03	.00
3	1	.00	.00	-.68	.37	-.01	.00	-.18	-.21	.00
4	6	.00	.00	.07	.10	.09	.00	-.18	.04	.00
5	1	.00	.00	-.01	.28	.03	.00	-.60	.15	.00
6	6	.00	.00	.23	-.17	-.11	.00	-.05	.23	.00
7	1	.00	.00	.36	-.29	-.06	.00	-.06	.23	.00
8	6	.00	.00	-.10	-.28	.08	.00	-.08	-.02	.00
9	1	.00	.00	-.25	-.57	.15	.00	.23	-.11	.00
10	1	.27	.04	-.21	-.15	.21	.00	-.23	-.17	-.01
11	1	-.27	-.04	-.21	-.15	.21	.00	-.23	-.17	.01

		7		8		9	
		A"		A'		A"	
Frequencies --		869.4566		1016.8431		1111.4624	
Red. masses --		1.2992		1.5681		1.1217	
Frc consts --		.5787		.9553		.8164	
IR Inten --		.2993		15.6044		43.8827	

Raman Activ --		9.4192			1.0896			.3929		
Depolar --		.7500			.1721			.7500		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	.00	.02	.03	.04	.00	.00	.00	-.03
2	8	.00	.00	-.01	-.02	.00	.00	.00	.00	.01
3	1	.00	.00	-.33	.04	.04	.00	.00	.00	.09
4	6	.00	.00	.12	.02	-.09	.00	.00	.00	.08
5	1	.00	.00	-.55	.18	-.14	.00	.00	.00	-.75
6	6	.00	.00	-.09	.10	.04	.00	.00	.00	.00
7	1	.00	.00	.54	.47	-.09	.00	.00	.00	-.57
8	6	.00	.00	-.04	-.14	.08	.00	.00	.00	.05
9	1	.00	.00	.18	.40	-.07	.00	.00	.00	-.08
10	1	-.32	-.04	.10	-.42	-.26	-.04	.21	.02	-.05
11	1	.32	.04	.10	-.42	-.26	.04	-.21	-.02	-.05
		10			11			12		
		A"			A'			A"		
Frequencies --		1142.2336			1164.9738			1193.7239		
Red. masses --		1.6975			3.2553			1.5751		
Frc consts --		1.3049			2.6030			1.3224		
IR Inten --		1.4072			30.6241			2.7001		
Raman Activ --		9.4777			4.1846			3.7028		
Depolar --		.7500			.3428			.7500		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	.00	-.22	.16	.12	.00	.00	.00	.03
2	8	.00	.00	.05	.03	-.04	.00	.00	.00	-.01
3	1	.00	.00	.90	.40	.07	.00	.00	.00	-.13
4	6	.00	.00	.08	-.23	-.05	.00	.00	.00	-.04
5	1	.00	.00	.04	-.04	-.12	.00	.00	.00	-.08
6	6	.00	.00	.01	-.24	-.09	.00	.00	.00	.17
7	1	.00	.00	.17	-.02	-.17	.00	.00	.00	-.57
8	6	.00	.00	-.05	.18	.11	.00	.00	.00	-.14
9	1	.00	.00	.10	.73	-.03	.00	.00	.00	.29
10	1	-.21	-.01	.06	.02	-.15	-.06	-.49	.03	.14
11	1	.21	.01	.06	.02	-.15	.06	.49	-.03	.14
		13			14			15		
		A'			A'			A'		
Frequencies --		1264.3070			1401.4381			1449.2135		
Red. masses --		2.0745			1.3656			1.3601		
Frc consts --		1.9537			1.5803			1.6830		
IR Inten --		62.7327			.3697			4.5993		
Raman Activ --		21.2858			.9333			27.2284		
Depolar --		.6369			.3286			.3322		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.14	.14	.00	-.02	-.01	.00	.03	.03	.00
2	8	-.03	-.02	.00	.02	.00	.00	.00	-.02	.00
3	1	.25	.12	.00	.24	-.07	.00	-.13	.07	.00
4	6	-.13	-.11	.00	-.12	-.01	.00	.00	-.14	.00
5	1	-.71	.05	.00	.77	-.27	.00	.26	-.23	.00
6	6	.11	.06	.00	-.02	.11	.00	.03	.09	.00
7	1	.18	.04	.00	.35	-.02	.00	-.81	.39	.00
8	6	-.04	-.10	.00	.01	-.08	.00	.01	.02	.00
9	1	-.49	.02	.00	-.23	-.01	.00	.01	.02	.00
10	1	.07	.12	.06	.11	.14	.06	-.08	-.01	.02
11	1	.07	.12	-.06	.11	.14	-.06	-.08	-.01	-.02

	16			17			18		
	A'			A'			A"		
Frequencies --	1557.5544			1567.5737			1622.8609		
Red. masses --	1.2106			1.2569			1.0451		
Frc consts --	1.7304			1.8197			1.6217		
IR Inten --	6.8221			.1848			7.2942		
Raman Activ --	5.4861			13.3307			17.0904		
Depolar --	.7398			.5744			.7500		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-.06	-.05	.00	-.02	-.02	.00	.00	.00	.00
2 8	-.02	.07	.00	-.01	.03	.00	.00	.00	.00
3 1	.81	-.29	.00	.39	-.13	.00	.00	.00	.00
4 6	.01	.00	.00	.01	-.03	.00	.00	.00	.00
5 1	-.07	.02	.00	-.06	-.01	.00	.00	.00	-.01
6 6	.03	-.03	.00	.03	.01	.00	.00	.00	.02
7 1	-.18	.04	.00	-.13	.07	.00	.00	.00	-.04
8 6	.06	.03	.00	-.13	.00	.00	.00	.00	.05
9 1	-.21	.09	.00	.42	-.14	.00	.00	.00	-.72
10 1	-.24	-.12	.07	.47	.06	-.26	-.27	-.41	-.05
11 1	-.24	-.12	-.07	.47	.06	.26	.27	.41	-.05

	19			20			21		
	A'			A'			A'		
Frequencies --	1628.8252			1878.7459			2006.5909		
Red. masses --	1.0575			5.4753			9.5583		
Frc consts --	1.6530			11.3866			22.6751		
IR Inten --	11.9496			28.1134			416.6209		
Raman Activ --	31.6933			72.6150			113.8721		
Depolar --	.6436			.2724			.3607		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.00	.01	.00	.03	-.05	.00	.53	-.44	.00
2 8	.01	-.01	.00	-.07	.06	.00	-.32	.32	.00
3 1	-.08	.03	.00	.11	-.08	.00	-.44	-.15	.00
4 6	-.03	.02	.00	.34	-.25	.00	-.11	.07	.00
5 1	.09	-.01	.00	-.40	-.11	.00	.26	-.06	.00
6 6	.01	.01	.00	-.37	.27	.00	.03	-.03	.00
7 1	.02	.00	.00	.56	.00	.00	-.07	.00	.00
8 6	.01	.05	.00	.07	-.02	.00	.00	.00	.00
9 1	-.43	.15	.00	-.22	.06	.00	.02	-.01	.00
10 1	.17	-.48	-.36	.12	-.07	-.05	.00	.01	.00
11 1	.17	-.48	.36	.12	-.07	.05	.00	.01	.00

	22			23			24		
	A'			A'			A"		
Frequencies --	3148.7327			3201.6705			3252.4057		
Red. masses --	1.0863			1.0380			1.1012		
Frc consts --	6.3456			6.2688			6.8631		
IR Inten --	96.2498			24.4022			25.4048		
Raman Activ --	72.2726			182.5467			119.8350		
Depolar --	.3129			.0459			.7500		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.02	.08	.00	.00	.00	.00	.00	.00	.00
2 8	.00	.00	.00	.00	.00	.00	.00	.00	.00
3 1	-.26	-.96	.00	.00	.01	.00	.00	.00	.00
4 6	.00	.00	.00	.00	.00	.00	.00	.00	.00
5 1	.00	.00	.00	.00	.01	.00	.00	.00	.00

```
  6   6      .00    .00    .00      .00    .00    .00      .00    .00    .00
  7   1      .02    .03    .00     -.01   -.03    .00      .00    .00    .00
  8   6      .00    .00    .00      .05   -.01    .00      .00    .00   -.09
  9   1      .00   -.01    .00     -.10   -.41    .00      .00    .00   -.02
 10   1      .00    .00   -.01     -.25    .28   -.52      .29   -.32    .56
 11   1      .00    .00    .01     -.25    .28    .52     -.29    .32    .56
                     25                     26                     27
                     A'                     A'                     A'
Frequencies --  3289.1477              3324.1110              3371.3767
Red. masses --     1.1015                 1.0910                 1.0933
Frc consts  --     7.0212                 7.1026                 7.3217
IR Inten    --    11.5451                28.6893                 6.4867
Raman Activ --    81.1477                51.8943                59.8360
Depolar     --      .7320                  .2038                  .2927
Atom AN      X      Y      Z        X      Y      Z        X      Y      Z
  1   6      .00    .00    .00      .00    .00    .00      .00    .00    .00
  2   8      .00    .00    .00      .00    .00    .00      .00    .00    .00
  3   1      .00   -.01    .00      .01    .03    .00      .00    .00    .00
  4   6      .00    .00    .00      .00    .01    .00      .02    .09    .00
  5   1     -.01   -.02    .00     -.01   -.02    .00     -.27   -.96    .00
  6   6      .01    .02    .00     -.02   -.08    .00      .01    .00    .00
  7   1     -.07   -.22    .00      .32    .91    .00     -.01   -.02    .00
  8   6      .00   -.09    .00      .00   -.02    .00      .00    .00    .00
  9   1      .22    .86    .00      .05    .19    .00     -.01   -.03    .00
 10   1     -.11    .11   -.23     -.04    .03   -.07      .00    .00    .00
 11   1     -.11    .11    .23     -.04    .03    .07      .00    .00    .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  8 AND MASS  15.99491
ATOM  3 HAS ATOMIC NUMBER  1 AND MASS   1.00783
ATOM  4 HAS ATOMIC NUMBER  6 AND MASS  12.00000
ATOM  5 HAS ATOMIC NUMBER  1 AND MASS   1.00783
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  6 AND MASS  12.00000
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
Molecular mass:    70.04186 amu.
Principle axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --    53.98101 820.13056 863.12449
          X            -.96187    .27350    .00000
          Y             .27350    .96187    .00000
          Z             .00000    .00000   1.00000
THIS MOLECULE IS AN ASYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER  1.
ROTATIONAL TEMPERATURES (KELVIN)      1.60452      .10561      .10035
ROTATIONAL CONSTANTS (GHZ)           33.43289     2.20055     2.09094
ZERO-POINT VIBRATIONAL ENERGY     253719.5 (JOULES/MOL)
```

```
                                  60.64043 (KCAL/MOL)
                                  .0966367 (HARTREE/PARTICLE)
 WARNING-- EXPLICIT CONSIDERATION OF   6 DEGREES OF FREEDOM AS
           VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
 VIBRATIONAL TEMPERATURES:    196.26   301.64   325.25   442.57   707.63
          (KELVIN)            839.93  1250.95  1463.00  1599.14  1643.41
                             1676.13  1717.49  1819.05  2016.35  2085.08
                             2240.96  2255.38  2334.92  2343.50  2703.08
                             2887.02  4530.30  4606.46  4679.46  4732.32
                             4782.63  4850.63
 SUM OF THERMAL ENERGIES:     .1022312 (HARTREE/PARTICLE)
 SUM OF HARTREE-FOCK AND THERMAL ENERGIES: -229.7017422 (HARTREE/PARTICLE)

 LEARN FROM YESTERDAY,
 LIVE FOR TODAY,
 LOOK TO TOMORROW,
 REST THIS AFTERNOON.

           -- SNOOPY
 Job cpu time:  0 days  0 hours 29 minutes 46.4 seconds.
newton.ncs.missouri.edu
```

PRINTOUT #2

```
*****************************************************
 Gaussian 92:  IBM-RS6000-G92/DFT-RevG.4  7-Sep-1994
                    4-Mar-1996
 *****************************************************
 %chk=croton
 Default route: MaxDisk=240000000 SCF=Direct
 ---------------------------------------------
 # rhf/6-31G* freq guess=read geom=checkpoint
 ---------------------------------------------
 1/10=4,29=10002,30=1/1,3;
 2/12=2,17=6,18=5/2;
 3/5=1,6=6,7=1,11=1,25=1,30=1/1,2,3;
 4/5=1,7=1/1;
 5/5=2/2;
 8/6=4,11=11,27=240000000/1;
 10/13=10/2;
 11/6=2,8=1,9=11,15=111,16=11/1,2,10;
 10/6=1,9=1/2;
 7/8=1,10=1,25=1/1,2,3,16;
 1/10=4,30=1/3;
 6/7=2,8=2,9=2,10=2,18=1,28=1/1;
 99//99;
 -----------------------------------------------------------
 Crotonaldehyde, staggered, Cs, rhf/6-31G* -- Frequencies
 -----------------------------------------------------------
 Z-Matrix taken from the checkpoint file:
 croton.chk
    Charge = 0 Multiplicity = 1
 C
 O,1,co
 H,1,hc1,2,hco
 C,1,cc1,2,cco,3,180.,0
 H,4,hca,1,hcca,2,0.,0
 C,4,cc2,1,ccc1,2,180.,0
 H,6,hc3,4,hccb,1,0.,0
 C,6,cc3,4,ccc2,1,180.,0
 H,8,hcip,7,hcipang,4,180.,0
 H,8,hcoop,7,hcoopang,4,di,0
 H,8,hcoop,7,hcoopang,4,-di,0
      Variables:
 co=1.19099929
 hc1=1.09554762
 cc1=1.4732206
 hca=1.07684599
 cc2=1.32424575
 hc3=1.0789592
 cc3=1.5067668
 hcip=1.0828162
 hcoop=1.0851074
 hco=120.62780174
 cco=124.17487621
```

```
hcca=116.44246849
ccc1=121.11785558
hccb=118.17108349
ccc2=125.10767665
hcipang=85.5694421
hcoopang=121.71564967
di=71.5699351
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                      ---------------------------
                      !   Initial Parameters    !
                      ! (Angstroms and Degrees) !
---------------------                           -----------------------
!      Name          Value   Derivative information (Atomic Units)     !
--------------------------------------------------------------------------
!       co          1.191    calculate D2E/DX2 analytically            !
!       hc1         1.0955   calculate D2E/DX2 analytically            !
!       cc1         1.4732   calculate D2E/DX2 analytically            !
!       hca         1.0768   calculate D2E/DX2 analytically            !
!       cc2         1.3242   calculate D2E/DX2 analytically            !
!       hc3         1.079    calculate D2E/DX2 analytically            !
!       cc3         1.5068   calculate D2E/DX2 analytically            !
!      hcip         1.0828   calculate D2E/DX2 analytically            !
!      hcoop        1.0851   calculate D2E/DX2 analytically            !
!       hco       120.6278   calculate D2E/DX2 analytically            !
!       cco       124.1749   calculate D2E/DX2 analytically            !
!      hcca       116.4425   calculate D2E/DX2 analytically            !
!      ccc1       121.1179   calculate D2E/DX2 analytically            !
!      hccb       118.1711   calculate D2E/DX2 analytically            !
!      ccc2       125.1077   calculate D2E/DX2 analytically            !
!     hcipang      85.5694   calculate D2E/DX2 analytically            !
!    hcoopang     121.7156   calculate D2E/DX2 analytically            !
!       di         71.5699   calculate D2E/DX2 analytically            !
--------------------------------------------------------------------------
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  28 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
--------------------------------------------------------------------------
                        Z-MATRIX (ANGSTROMS AND DEGREES)
CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
--------------------------------------------------------------------------
  1   1  C
  2   2  O     1   1.190999(  1)
  3   3  H     1   1.095548(  2)   2  120.628( 11)
  4   4  C     1   1.473221(  3)   2  124.175( 12)   3  180.000( 20)   0
  5   5  H     4   1.076846(  4)   1  116.442( 13)   2     .000( 21)   0
  6   6  C     4   1.324246(  5)   1  121.118( 14)   2  180.000( 22)   0
  7   7  H     6   1.078959(  6)   4  118.171( 15)   1     .000( 23)   0
  8   8  C     6   1.506767(  7)   4  125.108( 16)   1  180.000( 24)   0
  9   9  H     8   1.082816(  8)   7   85.569( 17)   4  180.000( 25)   0
 10  10  H     8   1.085107(  9)   7  121.716( 18)   4   71.570( 26)   0
 11  11  H     8   1.085107( 10)   7  121.716( 19)   4  -71.570( 27)   0
--------------------------------------------------------------------------
```

```
                Z-Matrix orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
Number     Number             X           Y           Z
---------------------------------------------------------------------
   1          6            .000000     .000000     .000000
   2          8            .000000     .000000    1.190999
   3          1            .942713     .000000    -.558137
   4          6          -1.218835     .000000    -.827538
   5          1          -2.157158     .000000    -.299195
   6          6          -1.148213     .000000   -2.149900
   7          1           -.171254     .000000   -2.607833
   8          6          -2.332890     .000000   -3.080967
   9          1          -2.020345     .000000   -4.117696
  10          1          -2.952540     .875722   -2.917862
  11          1          -2.952540    -.875722   -2.917862
---------------------------------------------------------------------
                   Distance matrix (angstroms):
             1          2          3          4          5
 1  C     .000000
 2  O    1.190999    .000000
 3  H    1.095548   1.987004    .000000
 4  C    1.473221   2.357977   2.178272    .000000
 5  H    2.177808   2.621833   3.110668   1.076846    .000000
 6  C    2.437306   3.532704   2.627867   1.324246   2.107861
 7  H    2.613450   3.802691   2.332848   2.065642   3.045263
 8  C    3.864549   4.867451   4.134520   2.513774   2.787318
 9  H    4.586634   5.680144   4.631433   3.386378   3.820951
10  H    4.242440   5.134893   4.637692   2.853432   2.873489
11  H    4.242440   5.134893   4.637692   2.853432   2.873489
             6          7          8          9         10
 6  C     .000000
 7  H    1.078959    .000000
 8  C    1.506767   2.212810    .000000
 9  H    2.152402   2.387221   1.082816    .000000
10  H    2.147615   2.932330   1.085107   1.753704    .000000
11  H    2.147615   2.932330   1.085107   1.753704   1.751444
            11
11  H     .000000
                         Interatomic angles:
      O2-C1-H3=120.6278       O2-C1-C4=124.1749       H3-C1-C4=115.1973
      C1-C4-H5=116.4425       C1-C4-C6=121.1179       H5-C4-C6=122.4397
      C4-C6-H7=118.1711       C4-C6-C8=125.1077       H7-C6-C8=116.7212
      C6-C8-H9=111.3881      C6-C8-H10=110.8608      H9-C8-H10=107.9835
     C6-C8-H11=110.8608      H9-C8-H11=107.9835     H10-C8-H11=107.6149
STOICHIOMETRY    C4H6O
FRAMEWORK GROUP  CS[SG(C4H4O),X(H2)]
DEG. OF FREEDOM   18
FULL POINT GROUP                 CS      NOP  2
LARGEST ABELIAN SUBGROUP         CS      NOP  2
LARGEST CONCISE ABELIAN SUBGROUP CS      NOP  2
                 Standard orientation:
---------------------------------------------------------------------
Center     Atomic              Coordinates (Angstroms)
```

```
Number     Number              X           Y           Z
---------------------------------------------------------------
   1          6          -1.446841     .049949     .000000
   2          8          -2.289503     .891614     .000000
   3          1          -1.718149   -1.011473     .000000
   4          6            .000000     .327494     .000000
   5          1            .289285    1.364755     .000000
   6          6            .885696    -.656970     .000000
   7          1            .519290   -1.671810     .000000
   8          6           2.381647    -.476756     .000000
   9          1           2.894287   -1.430534     .000000
  10          1           2.704145     .076927     .875722
  11          1           2.704145     .076927    -.875722
---------------------------------------------------------------
Rotational constants (GHZ):     33.2404822      2.1999538      2.0897703
Isotopes: C-12,O-16,H-1,C-12,H-1,C-12,H-1,C-12,H-1,H-1,H-1
Standard basis: 6-31G(D)     (S, S=P, 6D, 7F)
There are    65 symmetry adapted basis functions of A'  symmetry.
There are    22 symmetry adapted basis functions of A"  symmetry.
Crude estimate of integral set expansion from redundant integrals=1.829.
Integral buffers will be    262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
   87 basis functions      164 primitive gaussians
   19 alpha electrons       19 beta electrons
      nuclear repulsion energy       154.0345436915 Hartrees.
One-electron integrals computed using PRISM.
One-electron integral symmetry used in STVInt
The smallest eigenvalue of the overlap matrix is  3.233D-03
DipDrv:  MaxL=4.
DipDrv:  will hold 34 matrices at once.
Initial guess read from the checkpoint file:
croton.chk
Guess basis functions will be translated to current atomic coordinates.
INITIAL GUESS ORBITAL SYMMETRIES.
      OCCUPIED  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A") (A') (A") (A') (A') (A")
      VIRTUAL   (A") (A') (A") (A') (A') (A') (A") (A') (A') (A')
                (A') (A') (A') (A") (A') (A") (A') (A') (A") (A")
                (A') (A') (A') (A') (A') (A') (A") (A') (A') (A')
                (A') (A") (A') (A') (A') (A') (A") (A') (A") (A")
                (A') (A") (A') (A') (A') (A") (A') (A') (A") (A')
                (A') (A") (A') (A") (A') (A') (A") (A') (A") (A')
                (A') (A') (A') (A') (A') (A') (A') (A')
Alpha deviation from unit magnitude is 1.31D-14 for orbital   83.
Alpha deviation from orthogonality  is 8.42D-15 for orbitals  54  52.
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) =  -229.801048632     A.U. after    1 cycles
           Convg  =     .1336D-08             -V/T =  2.0013
           S**2   =    .0000
Range of M.O.s used for correlation:     1    87

     ***** edited for brevity *****
```

```
 Full mass-weighted force constant matrix:
 Low frequencies --- -203.0843   -4.7303   -3.6141    -.0016     .0012     .0023
 Low frequencies ---    5.5315  145.5182  224.0104
 ******    1 imaginary frequencies (negative signs) ******
 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:
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
                     A"                     A"                     A'
 Frequencies --  -203.0843               145.5182               224.0104
 Red. masses --     1.0939                 4.0919                 3.5471
 Frc consts  --      .0266                  .0511                  .1049
 IR Inten    --     1.1708                 4.3032                 8.6430
 Raman Activ --     3.3668                  .3919                  .1147
 Depolar     --      .7500                  .7500                  .6831
 Atom AN      X      Y      Z        X      Y      Z        X      Y      Z
   1   6      .00    .00    .03      .00    .00   -.15     -.09   -.05    .00
   2   8      .00    .00   -.01      .00    .00    .27      .13    .18    .00
   3   1      .00    .00    .14      .00    .00   -.31     -.34    .02    .00
   4   6      .00    .00   -.07      .00    .00   -.36     -.06   -.26    .00
   5   1      .00    .00   -.24      .00    .00   -.54     -.03   -.27    .00
   6   6      .00    .00    .04      .00    .00   -.03      .02   -.19    .00
   7   1      .00    .00    .23      .00    .00    .19      .20   -.25    .00
   8   6      .00    .00    .00      .00    .00    .17     -.02    .22    .00
   9   1      .00    .00   -.53      .00    .00    .44      .27    .38    .00
  10   1      .07   -.46    .27     -.15    .16    .13     -.19    .32    .00
  11   1     -.07    .46    .27      .15   -.16    .13     -.19    .32    .00
                      4                      5                      6
                     A"                     A'                     A'
 Frequencies --   317.4717               485.7135               583.0525
 Red. masses --     2.2137                 3.4281                 4.3426
 Frc consts  --      .1315                  .4765                  .8698
 IR Inten    --     9.3616                 3.5712                16.3935
 Raman Activ --      .7972                 6.2494                 2.2838
 Depolar     --      .7500                  .2535                  .3446
 Atom AN      X      Y      Z        X      Y      Z        X      Y      Z
   1   6      .00    .00   -.19     -.22   -.03    .00      .00    .26    .00
   2   8      .00    .00    .05     -.11    .10    .00     -.32   -.02    .00
   3   1      .00    .00   -.69     -.38    .01    .00      .17    .21    .00
   4   6      .00    .00    .08     -.11   -.09    .00      .18   -.05    .00
   5   1      .00    .00   -.02     -.30   -.03    .00      .61   -.16    .00
   6   6      .00    .00    .23      .16    .11    .00      .06   -.22    .00
   7   1      .00    .00    .38      .28    .06    .00      .09   -.24    .00
   8   6      .00    .00   -.10      .28   -.07    .00      .09    .02    .00
   9   1      .00    .00   -.23      .02   -.21    .00      .36    .17    .00
  10   1      .26    .03   -.21      .43   -.17    .00     -.07    .12    .00
  11   1     -.26   -.03   -.21      .43   -.17    .00     -.07    .12    .00
                      7                      8                      9
                     A"                     A'                     A"
 Frequencies --   867.8548              1059.6105              1103.4180
```

Red. masses --		1.3582			1.6552			1.1095		
Frc consts --		.6027			1.0949			.7959		
IR Inten --		.0446			1.0626			43.6528		
Raman Activ --		9.8418			1.8855			.4071		
Depolar --		.7500			.1594			.7500		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	.00	.02	.03	.04	.00	.00	.00	.00
2	8	.00	.00	-.01	-.02	.00	.00	.00	.00	.00
3	1	.00	.00	-.33	.03	.04	.00	.00	.00	-.03
4	6	.00	.00	.13	.03	-.10	.00	.00	.00	.08
5	1	.00	.00	-.51	.19	-.15	.00	.00	.00	-.76
6	6	.00	.00	-.11	.11	.05	.00	.00	.00	.00
7	1	.00	.00	.57	.44	-.06	.00	.00	.00	-.54
8	6	.00	.00	-.04	-.16	.08	.00	.00	.00	.06
9	1	.00	.00	.18	-.71	-.22	.00	.00	.00	-.12
10	1	-.33	-.04	.11	.16	-.19	.05	.23	.05	-.06
11	1	.33	.04	.11	.16	-.19	-.05	-.23	-.05	-.06
		10			11			12		
		A"			A'			A"		
Frequencies --		1137.9949			1153.8559			1191.0048		
Red. masses --		1.7313			2.7898			1.5281		
Frc consts --		1.3210			2.1884			1.2771		
IR Inten --		4.8770			6.3616			3.0696		
Raman Activ --		8.6801			4.0405			2.8804		
Depolar --		.7500			.2624			.7500		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.00	.00	.22	-.12	-.09	.00	.00	.00	-.06
2	8	.00	.00	-.05	-.03	.03	.00	.00	.00	.01
3	1	.00	.00	-.89	-.32	-.05	.00	.00	.00	.23
4	6	.00	.00	-.09	.18	.04	.00	.00	.00	.04
5	1	.00	.00	.12	-.07	.12	.00	.00	.00	.12
6	6	.00	.00	-.03	.23	.09	.00	.00	.00	-.16
7	1	.00	.00	.01	.07	.15	.00	.00	.00	.57
8	6	.00	.00	.06	-.16	-.13	.00	.00	.00	.12
9	1	.00	.00	-.11	.29	.12	.00	.00	.00	-.26
10	1	.22	.05	-.06	-.52	.15	-.05	.46	.13	-.13
11	1	-.22	-.05	-.06	-.52	.15	.05	-.46	-.13	-.13
		13			14			15		
		A'			A'			A'		
Frequencies --		1247.9950			1393.3889			1455.3913		
Red. masses --		2.3120			1.3305			1.3626		
Frc consts --		2.1216			1.5220			1.7005		
IR Inten --		102.2674			2.0160			4.7638		
Raman Activ --		20.6155			.5283			23.5329		
Depolar --		.6371			.2537			.3212		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	.17	.16	.00	-.02	-.02	.00	.03	.03	.00
2	8	-.02	-.02	.00	.03	.00	.00	.00	-.02	.00
3	1	.32	.13	.00	.22	-.08	.00	-.12	.07	.00
4	6	-.17	-.12	.00	-.11	.00	.00	-.01	-.14	.00
5	1	-.70	.02	.00	.78	-.25	.00	.28	-.23	.00
6	6	.09	.06	.00	-.03	.10	.00	.03	.09	.00
7	1	.25	.00	.00	.39	-.05	.00	-.80	.40	.00
8	6	-.02	-.09	.00	.01	-.07	.00	.02	.01	.00

9	1	.23	.05	.00	.22	.04	.00	-.08	-.03	.00	
10	1	-.26	.11	-.04	-.10	.10	-.06	-.07	.03	.02	
11	1	-.26	.11	.04	-.10	.10	.06	-.07	.03	-.02	
		16			17			18			
		A'			A'			A'			
Frequencies --		1554.5073			1566.7689			1632.7919			
Red. masses --		1.2018			1.2260			1.0594			
Frc consts --		1.7110			1.7731			1.6640			
IR Inten --		8.1449			1.5314			3.0715			
Raman Activ --		9.3018			4.7433			13.5718			
Depolar --		.7442			.5714			.7471			
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	-.05	-.04	.00	.04	.03	.00	.00	-.01	.00	
2	8	-.01	.06	.00	.02	-.05	.00	.00	.01	.00	
3	1	.71	-.26	.00	-.56	.20	.00	.03	-.02	.00	
4	6	.00	.00	.00	-.02	.03	.00	.02	.00	.00	
5	1	-.05	.02	.00	.08	.01	.00	-.04	.02	.00	
6	6	.03	-.02	.00	-.03	.00	.00	-.01	-.02	.00	
7	1	-.11	.02	.00	.20	-.09	.00	-.01	-.02	.00	
8	6	.07	.03	.00	.11	.02	.00	.04	-.04	.00	
9	1	-.27	-.15	.00	-.29	-.19	.00	-.44	-.28	.00	
10	1	-.32	-.09	.21	-.42	-.05	.22	.00	.50	-.32	
11	1	-.32	-.09	-.21	-.42	-.05	-.22	.00	.50	.32	
		19			20			21			
		A"			A'			A'			
Frequencies --		1635.8132			1873.0417			2005.6465			
Red. masses --		1.0445			5.6590			9.5559			
Frc consts --		1.6468			11.6974			22.6481			
IR Inten --		6.1365			25.8642			416.7662			
Raman Activ --		21.1679			71.0499			109.7203			
Depolar --		.7500			.2902			.3617			
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	.00	.00	.00	.03	-.05	.00	.53	-.44	.00	
2	8	.00	.00	.00	-.07	.06	.00	-.32	.32	.00	
3	1	.00	.00	.00	.12	-.09	.00	-.44	-.15	.00	
4	6	.00	.00	.00	.35	-.26	.00	-.11	.07	.00	
5	1	.00	.00	.00	-.42	-.11	.00	.26	-.06	.00	
6	6	.00	.00	-.02	-.38	.28	.00	.03	-.04	.00	
7	1	.00	.00	.01	.56	.00	.00	-.08	.01	.00	
8	6	.00	.00	-.05	.06	-.03	.00	.00	.00	.00	
9	1	.00	.00	.72	.20	.04	.00	-.01	.00	.00	
10	1	.35	-.34	.05	-.08	-.02	.05	.02	-.01	.00	
11	1	-.35	.34	.05	-.08	-.02	-.05	.02	-.01	.00	
		22			23			24			
		A'			A'			A"			
Frequencies --		3148.4033			3213.0870			3269.8952			
Red. masses --		1.0863			1.0374			1.1023			
Frc consts --		6.3440			6.3105			6.9443			
IR Inten --		97.7927			19.6770			19.4110			
Raman Activ --		74.5778			146.0865			76.4648			
Depolar --		.3111			.0131			.7500			
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z	
1	6	.02	.08	.00	.00	.00	.00	.00	.00	.00	
2	8	.00	.00	.00	.00	.00	.00	.00	.00	.00	

```
  3   1     -.27   -.96    .00      .00    .01    .00      .00    .00    .00
  4   6      .00    .00    .00      .00    .00    .00      .00    .00    .00
  5   1      .00    .00    .00      .00    .01    .00      .00    .00    .00
  6   6      .00    .00    .00      .00    .00    .00      .00    .00    .00
  7   1      .01    .03    .00      .00   -.02    .00      .00    .00    .00
  8   6      .00    .00    .00      .05    .02    .00      .00    .00    .09
  9   1      .00    .01    .00     -.21    .41    .00      .00    .00    .02
 10   1      .00    .00    .00     -.17   -.32   -.51     -.21   -.37   -.56
 11   1      .00    .00    .00     -.17   -.32    .51      .21    .37   -.56
                     25                    26                    27
                     A'                    A'                    A'
Frequencies --  3290.6019             3332.8440             3365.0649
Red. masses --     1.1022                1.0911                1.0932
Frc consts  --     7.0316                7.1407                7.2936
IR Inten    --    22.1217               22.4854                6.9641
Raman Activ --    75.3107               71.9405               58.3551
Depolar     --      .7478                 .3260                 .2802
Atom AN      X      Y      Z        X      Y      Z        X      Y      Z
  1   6      .00    .00    .00      .00    .00    .00      .00    .00    .00
  2   8      .00    .00    .00      .00    .00    .00      .00    .00    .00
  3   1      .00    .00    .00      .01    .03    .00      .00    .00    .00
  4   6      .00    .00    .00      .00    .01    .00     -.02   -.09    .00
  5   1      .00    .01    .00     -.01   -.03    .00      .27    .96    .00
  6   6      .00   -.02    .00     -.03   -.08    .00     -.01    .00    .00
  7   1      .07    .20    .00      .33    .92    .00      .01    .03    .00
  8   6     -.02    .09    .00      .01   -.02    .00      .00    .00    .00
  9   1      .40   -.77    .00     -.09    .17    .00      .00    .01    .00
 10   1     -.09   -.15   -.26      .02    .02    .04      .01    .01    .01
 11   1     -.09   -.15    .26      .02    .02   -.04      .01    .01   -.01
-------------------
- THERMOCHEMISTRY -
-------------------
TEMPERATURE   298.150 KELVIN.
PRESSURE      1.00000 ATM.
ATOM  1 HAS ATOMIC NUMBER  6 AND MASS  12.00000
ATOM  2 HAS ATOMIC NUMBER  8 AND MASS  15.99491
ATOM  3 HAS ATOMIC NUMBER  1 AND MASS   1.00783
ATOM  4 HAS ATOMIC NUMBER  6 AND MASS  12.00000
ATOM  5 HAS ATOMIC NUMBER  1 AND MASS   1.00783
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  6 AND MASS  12.00000
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
Molecular mass:    70.04186 amu.
Principle axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --    54.29347 820.35413 863.60745
          X             .96202   -.27299    .00000
          Y            -.27299   -.96202    .00000
          Z             .00000    .00000   1.00000
THIS MOLECULE IS AN ASYMMETRIC TOP.
ROTATIONAL SYMMETRY NUMBER  1.
```

```
ROTATIONAL TEMPERATURES (KELVIN)      1.59528      .10558      .10029
ROTATIONAL CONSTANTS (GHZ)           33.24048     2.19995     2.08977
   1 IMAGINARY FREQUENCIES IGNORED.
ZERO-POINT VIBRATIONAL ENERGY     252739.5 (JOULES/MOL)
                                  60.40620 (KCAL/MOL)
                                  .0962634 (HARTREE/PARTICLE)
WARNING-- EXPLICIT CONSIDERATION OF   5 DEGREES OF FREEDOM AS
          VIBRATIONS MAY CAUSE SIGNIFICANT ERROR
VIBRATIONAL TEMPERATURES:    209.37   322.30   456.77   698.83   838.88
         (KELVIN)           1248.64  1524.53  1587.56  1637.31  1660.13
                            1713.58  1795.58  2004.76  2093.97  2236.58
                            2254.22  2349.21  2353.56  2694.87  2885.66
                            4529.82  4622.89  4704.62  4734.41  4795.19
                            4841.55
SUM OF THERMAL ENERGIES:     .1012903 (HARTREE/PARTICLE)
SUM OF HARTREE-FOCK AND THERMAL ENERGIES: -229.6997583 (HARTREE/PARTICLE)

TRUST EVERYONE, BUT CUT THE CARDS.
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