ReOODCD22

```
                                          ***************************
                                          *  F R E Q U E N C I E S  *
                                          ***************************


  Coordinates (Cartesian)
  =======================

    Atom                      bohr
angstrom                 Geometric Variables
                      X           Y           Z              X
Y           Z       (0:frozen, *:LT par.)
  ---------------------------------------------------------------------------
--------------------------------
    1 Re        0.000685    0.004060    0.001991       0.000363
0.002149    0.001054      1       2       3
    2 O         3.670565   -0.017357   -0.006963       1.942379
-0.009185   -0.003684      4       5       6
    3 H         4.342721    1.699618   -0.049972       2.298068
0.899399   -0.026444      7       8       9
    4 O        -1.296761    0.113959   -2.956352      -0.686216
0.060304   -1.564433     10      11      12
    5 C        -0.782126   -3.012068    1.751271      -0.413883
-1.593917    0.926732     13      14      15
    6 H        -0.363896   -3.243920    3.768913      -0.192566
-1.716608    1.994422     16      17      18
    7 H        -1.731970   -4.613817    0.848562      -0.916519
-2.441526    0.449040     19      20      21
    8 C        -0.975917    2.804055    2.006299      -0.516433
1.483841    1.061687     22      23      24
    9 H        -1.917489    4.447000    1.167074      -1.014691
2.353251    0.617589     25      26      27
   10 H        -0.739884    2.885117    4.063941      -0.391530
1.526738    2.150544     28      29      30
  ---------------------------------------------------------------------------
--------------------------------


  Atomic Masses:
  --------------
     1. Re            186.95575000
     2. O              15.99491400
     3. H               2.00000000
     4. O              15.99491400
     5. C              12.00000000
     6. H               2.00000000
     7. H               2.00000000
     8. C              12.00000000
     9. H               2.00000000
    10. H               2.00000000



  ====================================
```

Normal Modes in Symmetry Displacements *** (cartesians, not mass-weighted) ***

==========

=== A ===

Symmetry Displacements

	1			2			3		
1.Re	0.037	0.000	0.000	0.000	0.037	0.000	0.000	0.000	0.037
2.O	-0.106	-0.001	-0.011	0.000	-0.097	0.000	0.001	0.000	-0.096
3.H	-0.106	-0.001	-0.013	-0.004	-0.095	-0.005	0.001	0.000	-0.094
4.O	-0.115	0.000	0.004	0.000	-0.119	0.000	0.009	0.001	-0.110
5.C	-0.102	0.000	0.003	0.008	-0.104	0.009	-0.004	0.000	-0.109
6.H	-0.096	0.000	0.001	0.009	-0.097	0.010	-0.010	-0.001	-0.108
7.H	-0.105	0.000	0.005	0.012	-0.109	0.014	-0.002	0.000	-0.112
8.C	-0.100	0.000	0.003	-0.007	-0.103	-0.008	-0.005	0.000	-0.109
9.H	-0.102	0.000	0.006	-0.012	-0.108	-0.013	-0.003	0.000	-0.111
10.H	-0.094	0.000	0.002	-0.008	-0.097	-0.008	-0.011	-0.001	-0.108

	4			5			6		
1.Re	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2.O	0.217	-0.001	-0.007	0.000	0.170	0.000	0.000	0.000	0.166
3.H	-0.070	-0.001	-0.008	0.053	-0.220	-0.004	0.014	0.000	-0.233
4.O	-0.076	0.000	0.003	0.003	-0.049	0.000	-0.115	0.002	-0.038
5.C	-0.067	0.000	0.002	-0.096	-0.053	0.008	0.049	-0.001	-0.057
6.H	-0.063	0.000	0.001	-0.104	-0.061	0.008	0.119	-0.002	-0.072
7.H	-0.070	0.001	0.004	-0.147	-0.025	0.012	0.017	0.000	-0.025
8.C	-0.065	0.000	0.003	0.088	-0.046	-0.007	0.058	-0.001	-0.047
9.H	-0.067	0.001	0.005	0.139	-0.019	-0.011	0.028	0.000	-0.014
10.H	-0.061	0.000	0.002	0.090	-0.048	-0.007			

```
0.129  -0.002  -0.055


                          7                          8
9
               ------------------------   ------------------------
------------------------
     1.Re         0.000   0.000   0.000      0.000   0.000   0.000
0.000   0.000   0.000
     2.O          0.000   0.000   0.000      0.000   0.000   0.000
0.000   0.000   0.000
     3.H         -0.231   0.010  -0.472     -0.005  -0.113  -0.047
0.049  -0.005   0.027
     4.O          0.105   0.002   0.041      0.000   0.156  -0.004
0.000   0.000   0.201
     5.C         -0.057  -0.001  -0.010      0.017  -0.079   0.105
0.003   0.000  -0.093
     6.H          0.127  -0.002  -0.048      0.014  -0.008   0.113
-0.047   0.003  -0.082
     7.H         -0.137  -0.002   0.076      0.028  -0.116   0.158
0.025  -0.001  -0.114
     8.C         -0.045  -0.002   0.014     -0.016  -0.072  -0.095
-0.002   0.000  -0.107
     9.H         -0.125  -0.003   0.101     -0.023  -0.106  -0.154
0.020  -0.001  -0.133
    10.H          0.142  -0.003  -0.008     -0.020   0.000  -0.098
-0.053   0.003  -0.101


                         10                         11
12
               ------------------------   ------------------------
------------------------
     1.Re         0.000   0.000   0.000      0.000   0.000   0.000
0.000   0.000   0.000
     2.O          0.000   0.000   0.000      0.000   0.000   0.000
0.000   0.000   0.000
     3.H          0.646   0.038  -0.180      0.000   0.629   0.008
0.000   0.000   0.373
     4.O          0.000   0.000   0.000      0.000   0.000   0.000
0.000   0.000   0.000
     5.C         -0.029  -0.001   0.004     -0.059  -0.045   0.023
-0.028  -0.001  -0.026
     6.H          0.046   0.001  -0.012     -0.072  -0.038   0.027
0.326   0.020  -0.097
     7.H         -0.050  -0.008   0.037     -0.088  -0.033   0.032
-0.175  -0.016   0.154
     8.C         -0.063  -0.002   0.013      0.060  -0.039  -0.024
-0.023   0.000  -0.047
     9.H         -0.105  -0.009   0.048      0.098  -0.026  -0.041
-0.180  -0.015   0.102
    10.H          0.011  -0.002   0.005      0.053  -0.028  -0.023
0.336   0.021  -0.089


                         13                         14
15
               ------------------------   ------------------------
------------------------
     1.Re         0.000   0.000   0.000      0.000   0.000   0.000
0.000   0.000   0.000
```

```
     2.O          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     3.H          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     4.O          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     5.C         -0.086  -0.003   0.014        -0.009  -0.045  -0.021
0.005   0.003  -0.094
     6.H          0.535  -0.022   0.076         0.000   0.677  -0.019
0.000   0.000   0.651
     7.H          0.013   0.024  -0.138        -0.006  -0.034  -0.043
-0.034   0.010  -0.066
     8.C          0.014   0.001   0.010         0.009  -0.046   0.023
-0.007  -0.001  -0.010
     9.H          0.181   0.027  -0.126         0.023  -0.036   0.026
-0.056   0.006   0.059
    10.H         -0.297  -0.014   0.046        -0.012  -0.063   0.025
0.098  -0.026  -0.021


                         16                        17
18
               ------------------------  ------------------------
------------------------
     1.Re         0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     2.O          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     3.H          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     4.O          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     5.C         -0.128  -0.004  -0.011         0.014  -0.049   0.014
0.006   0.006  -0.121
     6.H          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     7.H          0.601   0.012   0.067         0.000   0.679   0.029
0.000   0.000   0.585
     8.C          0.005   0.000  -0.007        -0.011  -0.049  -0.014
0.011   0.000   0.021
     9.H         -0.030   0.016   0.064        -0.024  -0.057  -0.016
0.112   0.029  -0.035
    10.H          0.168  -0.001  -0.026         0.003  -0.037  -0.016
-0.212  -0.060   0.049


                         19                        20
21
               ------------------------  ------------------------
------------------------
     1.Re         0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     2.O          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     3.H          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     4.O          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     5.C          0.025   0.004   0.003         0.020  -0.053   0.016
-0.001  -0.007   0.025
     6.H          0.000   0.000   0.000         0.000   0.000   0.000
```

```
0.000   0.000   0.000
     7.H          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     8.C         -0.148  -0.001  -0.015        -0.024  -0.053  -0.013
0.044   0.001  -0.109
     9.H          0.555  -0.043   0.124         0.000   0.675  -0.001
0.000   0.000   0.581
    10.H          0.184   0.025  -0.054         0.022  -0.039  -0.019
-0.261   0.035  -0.075


                          22                            23
24
               ------------------------      ------------------------
------------------------
     1.Re         0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     2.O          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     3.H          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     4.O          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     5.C          0.001   0.012   0.013        -0.003  -0.053  -0.040
0.007  -0.204  -0.009
     6.H          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     7.H          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     8.C         -0.014   0.017  -0.115         0.003  -0.054   0.004
-0.007   0.204   0.009
     9.H          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
    10.H          0.078  -0.179   0.615         0.000   0.641   0.212
0.000   0.000   0.000


  Frequencies and Normal Modes
  ============================

              1           2           3           4           5
6           7           8

           164.5773    196.4438    207.3276    211.7466    223.4127
265.7817    336.3697    423.0051
         ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1   -0.17021366  0.36395625 -0.01660522  0.13998159 -0.55193767
0.13124507 -0.00708626  0.06769714
    2    0.35956074 -0.02583571 -0.09746671 -0.12220167 -0.25873317
-0.52188198 -0.05760277 -0.00625618
    3    0.18388142  0.33753775  0.51974039  0.03431819  0.22126587
-0.10932016  0.02067994  0.01358143
    4   -0.10599531  0.22466802 -0.02194085  0.10133107 -0.38685470
0.10230525  0.01964778  0.16673722
    5   -0.18019552  0.01202980 -0.03414582  0.63031860  0.16796028
0.08882984 -0.18112455  0.03881718
    6    0.13881020 -0.63353026  0.04116209 -0.04717594 -0.28563715
0.32388642 -0.47577745  0.09962532
    7    0.25881247  0.32993385 -0.13474393 -0.05871075  0.20959504
0.22280537 -0.53537561 -0.37139821
```

```
    8   -0.16875125  0.08576777  0.08321295 -0.50188635  0.09527095
0.55344641  0.22282176 -0.03095482
    9    0.00083900 -0.01348482  0.45965352  0.06456220 -0.28382813
0.06377127  0.05733984  0.24027098
   10    0.09881280  0.21721316 -0.09067276 -0.17508307 -0.18701696
0.00429583 -0.18631752 -0.06929879
   11   -0.17499022 -0.00162470  0.00597843  0.37118355  0.16412443
0.19054549 -0.02932649  0.02498962
   12   -0.28385060 -0.29121466 -0.11827638  0.04783265 -0.06869489
-0.12331922  0.33892260 -0.51826783
   13   -0.47037997 -0.01804697  0.22921649 -0.20543129  0.06580945
-0.31598075 -0.32123974  0.05747974
   14   -0.09248019  0.07295789 -0.33651332 -0.13377882  0.09432561
0.05154430  0.03303496  0.33164267
   15    0.15194665  0.01026791 -0.09458750  0.07247815 -0.02081128
0.09255183  0.09779705 -0.00962343
   16    0.34270050 -0.06243538 -0.09555371  0.05518271  0.13022239
0.10817778  0.26688955  0.30558321
   17   -0.06579431  0.07707736 -0.03250750  0.07324087 -0.16272114
-0.01130305 -0.07671974 -0.27059415
   18   -0.37758106  0.03639217 -0.08076551 -0.21808166  0.10128765
-0.12842544 -0.19644025  0.18790846
   19   -0.03514003 -0.04049770  0.00575186 -0.02334417  0.14862744
-0.05119568 -0.10020831  0.25402037
   20   -0.00011266 -0.05857047 -0.00105272  0.00358689  0.14537558
-0.08874572 -0.08153737  0.22872323
   21    0.00473506  0.01948722 -0.15634510  0.02887364  0.01941240
-0.07605262 -0.00784486  0.07168024
   22    0.00102798  0.01718031 -0.10210018  0.01454812  0.01467417
-0.02865555 -0.00446116  0.06467616
   23    0.01511232 -0.06522881  0.33089084 -0.03263922 -0.03572339
0.08356011  0.01682674 -0.20580626
   24    0.09906892 -0.16016677  0.34973534  0.01689275  0.08580398
-0.01356117 -0.00553154 -0.03864811

              9          10          11          12          13
14          15          16

           474.9881    504.7805    584.0024    609.9796    630.3503
661.8129    689.6827    696.1466
         ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1   -0.01327123  0.09711039  0.14082557  0.48201839  0.33138555
-0.16834672 -0.20185857 -0.01562410
    2   -0.15514959 -0.02587351 -0.07149355  0.02564331  0.02316953
-0.19957652  0.08257842  0.61643738
    3   -0.02582655  0.22997317 -0.00571165  0.00155627  0.03223333
0.03538097  0.41821227 -0.02758752
    4   -0.02319247  0.12403635 -0.05831054 -0.50596388 -0.22682404
0.54610971 -0.12828832  0.23409808
    5   -0.10319206 -0.01043182 -0.10058522 -0.22686660  0.06486112
-0.42615375  0.05372582  0.13818729
    6   -0.00841677  0.08883085  0.05833318  0.01257410  0.03243508
0.01461675  0.20586752 -0.00657072
    7   -0.07847707  0.26628475  0.14622500  0.09184971  0.12709136
0.23398070 -0.03625346  0.12361085
    8    0.15675110 -0.02519521 -0.06474859 -0.06171455  0.02432464
-0.26115027  0.06196956  0.41884748
    9    0.00233671  0.23883607 -0.01300865  0.02232088 -0.00212897
-0.03933603  0.28267170 -0.03900212
   10    0.01150325  0.14612647 -0.23452465 -0.54632252  0.13408819
```

```
-0.43935335 -0.06574750 -0.31589976
   11   -0.05298503 -0.02595402  0.04664813  0.02785968 -0.04761475
0.04827786  0.03866533  0.36985381
   12   -0.07378522  0.52678289 -0.02691760 -0.09001898  0.30231709
0.09563589  0.13514353  0.04095790
   13    0.10536254 -0.12708631  0.40994414 -0.18352405  0.23947912
0.05890926  0.01208565 -0.00077708
   14   -0.48765217  0.19443331 -0.08666745  0.12375201 -0.08095611
0.06389535  0.31417686 -0.22166750
   15    0.02571549  0.05394652 -0.13552005  0.06691460 -0.07772070
-0.00102135  0.03496632 -0.02937792
   16   -0.07335678  0.04834833  0.42076338 -0.22028294  0.42052982
0.02209215 -0.09900414  0.01645413
   17    0.26039392 -0.22065251 -0.21571308  0.08058303 -0.10621548
0.08359156  0.29454173 -0.09584075
   18   -0.29405293  0.20062052 -0.07026076  0.09121505 -0.19012157
-0.11164427 -0.07424983  0.13010300
   19    0.15981672 -0.00822954 -0.54035106  0.06923190  0.47553417
0.22318989 -0.06418039  0.07686011
   20    0.30909746  0.24865920 -0.28825052  0.09563626  0.12375795
0.08516696 -0.23347302  0.00866572
   21    0.31281659  0.26253195  0.20701537  0.03871902 -0.26193873
-0.06699843 -0.15913292 -0.12509648
   22    0.16752895  0.09228804  0.05516703  0.00791093 -0.04469178
-0.03437337  0.08008327  0.02849870
   23   -0.51749889 -0.24958627 -0.17219324 -0.01745875  0.11130205
0.10884295 -0.34250704 -0.12025555
   24   -0.02609024  0.36843482 -0.03741133  0.08163102 -0.29128112
-0.13942719 -0.44367254  0.03570007

             17          18          19          20          21
22          23          24

           983.1411   1023.9865   1031.1573   2182.3215   2186.6274
2309.4758   2315.5641   2679.5966
         ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1   -0.22034817  0.00829664  0.05100380 -0.00155390  0.00609885
0.00060803  0.00130237 -0.00238024
    2    0.02211615  0.20772961 -0.03636148  0.01694303  0.00264947
-0.00116454  0.00163499  0.00145910
    3   -0.51235242 -0.02489407 -0.15695818  0.00175443 -0.01062925
0.00180423  0.00177974  0.00056453
    4   -0.13861462  0.01310635  0.03566451 -0.00047927  0.00541314
0.00054898  0.00055813  0.14924645
    5    0.01162140  0.10963958 -0.02049310  0.00895992  0.00055596
-0.00208971  0.00175310  0.45354139
    6   -0.29933284 -0.01063902 -0.08768357  0.00179764 -0.00632971
0.00054156  0.00141504 -0.00325511
    7    0.28541551  0.00052856  0.01906791  0.00025519 -0.00046714
-0.00159908 -0.00179620  0.09061723
    8   -0.02812286  0.18934619 -0.03295664  0.01785316  0.00269363
0.00127866  0.00013053  0.14155339
    9    0.69962275 -0.01910338 -0.08681956  0.00240870 -0.01492182
0.00018900 -0.00139671 -0.02068180
   10   -0.01735093 -0.01581503  0.02891410 -0.00179323  0.00302224
-0.00111400  0.00021130 -0.37173364
   11   -0.00080773  0.10950702 -0.01985997  0.00862928  0.00340609
-0.00078768  0.00135345 -0.77784349
   12   -0.02675251  0.00118933 -0.04311979  0.00111819 -0.00387225
-0.00091617 -0.00206646  0.00977215
```

```
   13    0.01520280  0.29509398  0.18797617 -0.12051385 -0.14901781
-0.02567093  0.15169233 -0.00063915
   14   -0.01134034  0.45610942  0.23945785  0.04722854  0.05305282
0.01292145 -0.06872302  0.00000377
   15   -0.00814723  0.06940253  0.03804590 -0.46462646 -0.57279698
-0.11559543  0.58799805 -0.00059440
   16    0.01477436 -0.03660246 -0.03022982  0.18522979  0.23802543
-0.08376056  0.38995503  0.00108687
   17    0.02049897  0.20603794  0.06456341  0.32313944  0.40301431
-0.10690836  0.51822661  0.00046870
   18   -0.00920623 -0.48847136 -0.29177230  0.09113783  0.11794190
-0.07256447  0.37289371 -0.00025548
   19    0.02311969 -0.01605049 -0.00206019 -0.29739504  0.23331947
0.37794407  0.04892188  0.00040761
   20   -0.01235647  0.17665782 -0.07780651  0.43359633 -0.28271820
-0.51689916 -0.09636353 -0.00098238
   21   -0.00210216  0.41297299 -0.59238793 -0.17580148  0.16885465
0.23755725  0.02070768 -0.00039622
   22   -0.00819494 -0.09192805  0.12997925  0.51314815 -0.40874732
0.68112553  0.11829229 -0.00138537
   23    0.01432408  0.29638269 -0.35512539  0.21849227 -0.14597878
0.14443939  0.11802685  0.00037525
   24   -0.06817425  0.12148733  0.51541923 -0.03372499  0.24927779
0.10406441  0.16369378  0.00171834


  Intensities
  ===========

                Frequency       Dipole Strength        Absorption
Intensity (degeneracy not counted)
                  cm-1           1e-40 esu2 cm2          km/mole
              ----------          ----------          ----------
              164.577311          162.265910            6.693840
              196.443803           27.540941            1.356111
              207.327610           43.780685            2.275191
              211.746625           79.436646            4.216144
              223.412683           39.400367            2.206410
              265.781713          148.688893            9.905621
              336.369707          386.792538           32.611670
              423.005069           10.044468            1.065002
              474.988109           10.776204            1.283000
              504.780522           16.790970            2.124499
              584.002434           68.218422            9.986065
              609.979622           51.771311            7.915577
              630.350347          705.660739          111.495162
              661.812903          408.050741           67.690461
              689.682674           33.819982            5.846565
              696.146593          147.940366           25.814604
              983.141109          444.860559          109.627076
             1023.986469           49.088791           12.599538
             1031.157288           48.179317           12.452703
             2182.321496            8.408087            4.599324
             2186.627404            6.288886            3.446883
             2309.475809            0.249693            0.144543
             2315.564141            0.544441            0.315999
             2679.596624           80.880678           54.324067


  Zero-Point Energy :      0.049191 a.u.
```

```
  ==================      1.338551 eV


  ============================
  Vibrations and Normal Modes  ***  (cartesian coordinates, NOT
mass-weighted)  ***
  ============================

  The headers on the normal mode eigenvectors below give the Frequency in cm-1
  (a negative value means an imaginary frequency, no output for
(almost-)zero frequencies)


                        164.577                     196.444
207.328
               ------------------------     ------------------------
------------------------
     1.Re        -0.010   0.021   0.011        -0.031   0.002  -0.029
-0.001  -0.006   0.034
     2.O         -0.008  -0.104   0.013        -0.024  -0.009   0.325
-0.005   0.007  -0.076
     3.H          0.028  -0.126  -0.459        -0.042   0.000   0.451
-0.006   0.008  -0.023
     4.O          0.064  -0.095  -0.024        -0.116  -0.036   0.001
-0.019   0.047   0.049
     5.C          0.069  -0.036  -0.036         0.213  -0.064  -0.033
0.031  -0.120  -0.146
     6.H         -0.379  -0.120   0.043         0.407  -0.103  -0.078
0.084  -0.396  -0.190
     7.H          0.438  -0.085  -0.346         0.246  -0.100  -0.004
0.026  -0.006  -0.351
     8.C         -0.019   0.025  -0.012         0.233   0.084  -0.015
0.010   0.132  -0.149
     9.H         -0.275  -0.031   0.174         0.235   0.113   0.040
0.162   0.035  -0.526
    10.H          0.387   0.021  -0.054         0.468   0.129  -0.044
-0.220   0.464  -0.140


                        211.747                     223.413
265.782
               ------------------------     ------------------------
------------------------
     1.Re         0.010  -0.009   0.003        -0.051  -0.024   0.020
-0.010   0.041   0.009
     2.O          0.014   0.237  -0.027        -0.062   0.134  -0.147
-0.017  -0.139  -0.132
     3.H         -0.162   0.311   0.216        -0.206   0.191  -0.111
0.142  -0.190   0.510
     4.O         -0.045  -0.189   0.022         0.370   0.092  -0.162
0.080  -0.308  -0.044
     5.C         -0.193   0.005  -0.051         0.044  -0.040   0.043
0.040   0.005  -0.086
     6.H         -0.477  -0.243  -0.028         0.136   0.167   0.053
0.388  -0.152  -0.178
     7.H         -0.249   0.189  -0.332         0.258  -0.249   0.194
-0.030   0.061  -0.107
     8.C          0.144   0.027   0.012         0.177   0.052   0.020
-0.017   0.007   0.099
     9.H          0.096   0.079   0.174         0.549   0.288   0.067
```

```
0.208   0.162   0.146
    10.H          0.358  -0.061  -0.003         0.205  -0.057   0.023
-0.374  -0.217   0.151


                      336.370                     423.005
474.988
               ------------------------     ------------------------
------------------------
     1.Re         0.000   0.003  -0.001         0.004   0.000   0.001
0.001   0.010   0.002
     2.O         -0.008   0.039   0.126         0.044   0.011   0.020
0.006   0.004  -0.002
     3.H         -0.002   0.018  -0.795         0.052   0.005  -0.037
-0.039   0.023  -0.010
     4.O          0.004  -0.075  -0.007        -0.106  -0.010   0.043
0.007  -0.079   0.000
     5.C         -0.019  -0.008  -0.060        -0.029   0.011  -0.051
-0.069  -0.060  -0.174
     6.H          0.271  -0.084  -0.129        -0.319   0.319   0.046
-0.067   0.519  -0.103
     7.H         -0.314   0.114   0.036         0.464  -0.268  -0.066
-0.013  -0.333   0.265
     8.C          0.014  -0.009   0.054        -0.008  -0.014  -0.030
0.061  -0.052   0.147
     9.H          0.258   0.111   0.011         0.487   0.257  -0.049
-0.103  -0.337  -0.245
    10.H         -0.187  -0.080   0.079        -0.319  -0.267   0.015
0.088   0.503   0.119


                      504.781                     584.002
609.980
               ------------------------     ------------------------
------------------------
     1.Re        -0.006   0.002  -0.015        -0.009   0.005   0.000
-0.036  -0.002   0.000
     2.O         -0.030  -0.001   0.016         0.047   0.017  -0.016
0.325   0.082  -0.001
     3.H         -0.043   0.003  -0.014         0.345  -0.100   0.081
0.808  -0.106  -0.042
     4.O          0.002  -0.001  -0.055         0.006  -0.006  -0.004
0.019   0.003  -0.017
     5.C          0.067   0.119   0.164         0.196  -0.095  -0.030
-0.136   0.029   0.054
     6.H         -0.225  -0.266   0.175        -0.379   0.098   0.115
0.270  -0.193  -0.055
     7.H          0.214   0.288  -0.298        -0.441   0.191   0.128
0.186  -0.118  -0.031
     8.C          0.076  -0.149   0.179        -0.174  -0.083   0.017
0.028  -0.030   0.004
     9.H          0.282  -0.309  -0.375         0.410   0.211  -0.064
-0.078  -0.121  -0.050
    10.H         -0.254   0.319   0.193         0.344   0.155  -0.053
0.093   0.045  -0.007


                      630.350                     661.813
689.683
               ------------------------     ------------------------
------------------------
```

```
     1.Re        -0.023  -0.002  -0.002        -0.012  -0.014   0.002
-0.014   0.006   0.028
     2.O          0.160  -0.017  -0.001         0.257  -0.101  -0.006
-0.011   0.003  -0.005
     3.H         -0.077   0.081  -0.026        -0.716   0.298   0.018
0.018  -0.011   0.001
     4.O          0.021   0.003  -0.001         0.000   0.009  -0.001
0.017  -0.004   0.000
     5.C          0.196  -0.092  -0.024         0.014   0.138  -0.051
0.067   0.138  -0.117
     6.H         -0.440   0.111   0.135         0.174   0.166  -0.090
0.128   0.367  -0.122
     7.H         -0.302   0.134   0.093         0.027   0.224  -0.193
-0.085   0.305  -0.212
     8.C          0.215   0.133  -0.003        -0.131   0.021   0.050
0.097  -0.189  -0.170
     9.H         -0.340  -0.130   0.096         0.103   0.184   0.089
-0.010  -0.374  -0.353
    10.H         -0.565  -0.185   0.102         0.159   0.217   0.014
0.192  -0.486  -0.195


                      696.147                     983.141
1023.986
               ------------------------    ------------------------
------------------------
     1.Re        -0.001   0.042  -0.002         0.034  -0.003   0.078
-0.001  -0.014   0.002
     2.O          0.096  -0.067   0.000         0.029   0.000  -0.011
-0.003   0.003  -0.001
     3.H         -0.452   0.157  -0.010         0.022   0.011   0.000
0.016  -0.005   0.004
     4.O         -0.004  -0.026  -0.001        -0.392   0.032  -0.895
0.001   0.001   0.002
     5.C         -0.064  -0.194   0.101        -0.007  -0.051  -0.018
0.063   0.239  -0.142
     6.H         -0.051  -0.431   0.092         0.001   0.037  -0.004
-0.250  -0.478  -0.162
     7.H         -0.084  -0.343   0.341        -0.080  -0.059   0.036
0.076  -0.143   0.540
     8.C          0.010  -0.157  -0.079        -0.010   0.063  -0.005
-0.050   0.136   0.094
     9.H          0.164  -0.186  -0.276        -0.103   0.041   0.020
-0.019  -0.068  -0.347
    10.H          0.109  -0.275  -0.100         0.020  -0.046   0.002
0.165  -0.305   0.086


                     1031.157                    2182.321
2186.627
               ------------------------    ------------------------
------------------------
     1.Re         0.003  -0.002  -0.010         0.000  -0.001   0.000
0.000   0.000   0.001
     2.O          0.004   0.000  -0.001         0.000   0.000   0.000
-0.001   0.000   0.000
     3.H          0.004   0.001   0.006         0.001   0.000   0.001
-0.001  -0.002   0.000
     4.O          0.004   0.000   0.008         0.000  -0.001   0.000
0.001   0.000   0.002
     5.C         -0.039  -0.150   0.094         0.016   0.066  -0.050
```

```
0.022   0.086  -0.062
     6.H          0.145   0.290   0.113         0.096  -0.047   0.459
0.121  -0.057   0.565
     7.H         -0.040   0.088  -0.338        -0.183  -0.307  -0.182
-0.235  -0.392  -0.231
     8.C         -0.081   0.221   0.162        -0.031   0.080   0.063
0.026  -0.066  -0.050
     9.H         -0.017  -0.106  -0.563         0.238  -0.415   0.223
-0.195   0.335  -0.179
    10.H          0.248  -0.477   0.159        -0.067  -0.013  -0.562
0.055   0.010   0.443


                      2309.476                    2315.564
2679.597
               ------------------------    ------------------------
------------------------
     1.Re         0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     2.O          0.000   0.000   0.000         0.000   0.000   0.000
-0.049  -0.114   0.002
     3.H         -0.001   0.000   0.000        -0.001   0.000   0.001
0.371   0.920  -0.018
     4.O         -0.001   0.001   0.000         0.001   0.000   0.001
0.000   0.000   0.001
     5.C          0.016   0.018   0.029         0.077   0.083   0.153
0.000   0.001   0.000
     6.H         -0.022   0.015  -0.119        -0.124   0.077  -0.610
0.000   0.000   0.001
     7.H         -0.071  -0.117  -0.063        -0.335  -0.568  -0.312
-0.001   0.000  -0.001
     8.C         -0.066   0.088  -0.155         0.012  -0.017   0.033
0.001   0.000  -0.001
     9.H          0.322  -0.561   0.278        -0.060   0.108  -0.054
0.001   0.001  -0.001
    10.H          0.070   0.031   0.651        -0.017  -0.007  -0.137
-0.001  -0.001   0.001
```

List of All Frequencies:

Intensities
==========

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
164.577311	162.265910	6.693840
196.443803	27.540941	1.356111
207.327610	43.780685	2.275191
211.746625	79.436646	4.216144
223.412683	39.400367	2.206410
265.781713	148.688893	9.905621
336.369707	386.792538	32.611670
423.005069	10.044468	1.065002
474.988109	10.776204	1.283000
504.780522	16.790970	2.124499

```
               584.002434           68.218422            9.986065
               609.979622           51.771311            7.915577
               630.350347          705.660739          111.495162
               661.812903          408.050741           67.690461
               689.682674           33.819982            5.846565
               696.146593          147.940366           25.814604
               983.141109          444.860559          109.627076
              1023.986469           49.088791           12.599538
              1031.157288           48.179317           12.452703
              2182.321496            8.408087            4.599324
              2186.627404            6.288886            3.446883
              2309.475809            0.249693            0.144543
              2315.564141            0.544441            0.315999
              2679.596624           80.880678           54.324067


  ============================
  Statistical Thermal Analysis  ***  ideal gas assumed  ***
  ============================

  Pressure:                  1.000000 atm.
  Temperature:             298.150000 K


  Moments of Inertia (and direction vectors)
  ==========================================

          601.0391        618.6538        642.0294
  ------------------------------------------------
           -0.2125         -0.9675         -0.1371
           -0.9770          0.2129          0.0113
           -0.0182         -0.1364          0.9905


      Temp
Transl     Rotat    Vibrat     Total
      ----
------     -----    ------     -----

      298.15   Entropy (cal/mole-K):
42.484    26.970    18.359    87.814
               Internal Energy (Kcal/mole):
0.889     0.889    34.211    35.989
               Constant Volume Heat Capacity (cal/mole-K):
2.981     2.981    23.239    29.200

********************************************************************************
```