ReOOHCH22

****
* 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	1.00782500
4. O	15.99491400
5. C	12.00000000
6. H	1.00782500
7. H	1.00782500
8. C	12.00000000
9. H	1.00782500
10. H	1.00782500

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

=== A ===

Symmetry Displacements

	1			2			3		
1.Re	0.036	0.000	0.000	0.000	0.036	0.000	0.000	0.000	0.036
2.O	-0.111	0.000	-0.005	0.000	-0.100	0.000	0.000	0.000	-0.099
3.H	-0.111	0.000	-0.007	-0.006	-0.098	-0.003	0.001	0.000	-0.097
4.O	-0.116	0.000	0.002	0.000	-0.121	0.000	0.010	0.000	-0.116
5.C	-0.109	0.000	0.001	0.010	-0.112	0.005	-0.005	0.000	-0.114
6.H	-0.106	0.000	0.001	0.011	-0.107	0.005	-0.012	0.000	-0.113
7.H	-0.110	0.000	0.003	0.015	-0.116	0.007	-0.002	0.000	-0.118
8.C	-0.108	0.000	0.002	-0.009	-0.112	-0.004	-0.006	0.000	-0.115
9.H	-0.109	0.000	0.003	-0.015	-0.116	-0.007	-0.004	0.000	-0.118
10.H	-0.105	0.000	0.001	-0.009	-0.108	-0.004	-0.013	0.000	-0.114

	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	0.215	-0.001	-0.004	0.000	0.158	0.000	0.000	0.000	0.157
3.H	-0.076	-0.001	-0.005	0.066	-0.263	-0.004	-0.009	0.000	-0.267
4.O	-0.080	0.000	0.002	0.004	-0.050	0.000	-0.125	0.000	-0.041
5.C	-0.075	0.000	0.001	-0.118	-0.059	0.007	0.063	0.000	-0.062
6.H	-0.073	0.000	0.001	-0.127	-0.070	0.008	0.144	0.000	-0.079
7.H	-0.076	0.000	0.002	-0.181	-0.024	0.011	0.027	0.000	-0.024
8.C	-0.074	0.000	0.001	0.109	-0.050	-0.007	0.074	0.000	-0.054
9.H	-0.074	0.000	0.002	0.174	-0.015	-0.010	0.040	0.000	-0.016
10.H	-0.071	0.000	0.001	0.113	-0.055	-0.007	0.156	0.000	-0.064

	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	-0.313	0.021	-0.710	-0.012	-0.132	-0.075	0.079	-0.008	0.093
4.O	0.080	-0.001	0.048	0.000	0.146	-0.004	0.000	0.000	0.194
5.C	-0.051	0.001	-0.021	0.016	-0.087	0.123	0.003	0.000	-0.103
6.H	0.221	0.002	-0.077	0.020	-0.002	0.131	-0.078	0.003	-0.086
7.H	-0.166	-0.003	0.107	0.024	-0.128	0.189	0.037	-0.001	-0.138
8.C	-0.040	0.000	0.005	-0.015	-0.077	-0.113	-0.002	0.000	-0.121
9.H	-0.160	-0.004	0.132	-0.026	-0.117	-0.179	0.033	0.000	-0.162
10.H	0.236	0.001	-0.027	-0.013	0.007	-0.117	-0.084	0.004	-0.112

	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	0.925	0.038	-0.253	0.000	0.926	0.015	0.000	0.000	0.534
4.O	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5.C	-0.022	0.000	0.002	-0.053	-0.037	0.020	-0.023	-0.001	-0.021
6.H	0.080	0.003	-0.018	-0.068	-0.031	0.024	0.472	0.026	-0.120
7.H	-0.054	-0.008	0.050	-0.079	-0.026	0.027	-0.227	-0.021	0.229
8.C	-0.053	-0.002	0.011	0.054	-0.032	-0.021	-0.018	0.000	-0.040
9.H	-0.108	-0.009	0.058	0.090	-0.020	-0.038	-0.239	-0.019	0.172
10.H	0.048	0.000	0.000	0.045	-0.022	-0.020	0.483	0.026	-0.098

	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         -0.071  -0.002   0.011        -0.007  -0.036  -0.019
0.004   0.002  -0.076
     6.H          0.775  -0.025   0.098         0.000   0.971  -0.015
0.000   0.000   0.945
     7.H          0.083   0.027  -0.202        -0.001  -0.026  -0.043
-0.047   0.007  -0.033
     8.C          0.014   0.001   0.008         0.007  -0.037   0.020
-0.005  -0.001  -0.005
     9.H          0.232   0.029  -0.181         0.023  -0.028   0.020
-0.065   0.003   0.072
    10.H         -0.421  -0.018   0.059        -0.019  -0.052   0.024
0.125  -0.021  -0.019


                          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         -0.097  -0.003  -0.009         0.011  -0.038   0.012
0.004   0.004  -0.093
     6.H          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     7.H          0.893   0.007   0.103         0.000   0.974   0.028
0.000   0.000   0.866
     8.C          0.007   0.001  -0.005        -0.010  -0.038  -0.012
0.009  -0.001   0.022
     9.H         -0.066   0.010   0.095        -0.025  -0.045  -0.010
0.153   0.027  -0.084
    10.H          0.238   0.004  -0.032         0.011  -0.028  -0.015
-0.309  -0.054   0.060


                          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          0.020   0.003   0.003         0.015  -0.040   0.011
0.000  -0.004   0.019
     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
```

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     8.C         -0.115  -0.001  -0.011        -0.017  -0.040  -0.010
0.032   0.002  -0.088
     9.H          0.842  -0.039   0.162         0.000   0.972   0.005
0.000   0.000   0.859
    10.H          0.294   0.025  -0.059         0.030  -0.029  -0.016
-0.377   0.023  -0.042


                         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   0.010   0.010        -0.002  -0.038  -0.029
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         -0.010   0.014  -0.085         0.002  -0.039   0.003
-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          0.115  -0.278   0.900         0.000   0.924   0.305
0.000   0.000   0.000


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

              1           2           3           4           5
6           7           8

           201.4955    209.9891    237.2318    240.8274    247.0381
311.7918    449.5951    566.2521
         ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1   -0.30511020 -0.09730592  0.40772177  0.37593849  0.33139582
0.11585682  0.02926495  0.12899943
    2    0.50765495 -0.05006884  0.23756288  0.27046743 -0.00834747
-0.40638170  0.01620096  0.00121388
    3    0.11877139 -0.49814970 -0.29753301 -0.14774703  0.36654096
-0.07447217  0.00527169 -0.09817623
    4   -0.20232451 -0.04437131  0.28997057  0.27872700  0.23403745
0.10539374 -0.03294611 -0.34811186
    5   -0.35628146  0.02708552 -0.53102213  0.41702310 -0.09159215
0.10780135  0.13925624 -0.02435396
    6    0.23266542  0.74652358 -0.00505567  0.01352141  0.17893201
0.21616138  0.35750484 -0.08387798
    7    0.14163735 -0.29573123  0.00950891  0.01061494 -0.12155590
0.29993594  0.61371332  0.21410467
    8   -0.18831317 -0.01967324  0.24229810 -0.57793229  0.03799845
0.43246559 -0.13370214  0.04450109
    9   -0.00610563  0.06334051 -0.03938473  0.02427977  0.59867118
```

```
0.01172093 -0.09333498 -0.22976897
   10    0.06451236 -0.12284872  0.23693656  0.03115673  0.01121258
0.04723924  0.21316824  0.01489474
   11   -0.22144077  0.02638590 -0.25753732  0.11522842 -0.03665631
0.12658371 -0.00509471 -0.02423248
   12   -0.16837486  0.24506547 -0.00982350 -0.01107236 -0.07384740
-0.21775185 -0.39131399  0.31425164
   13   -0.28798500  0.05526609  0.00408466 -0.23697704  0.11056980
-0.46994000  0.30361937 -0.03380301
   14   -0.08904072 -0.01706139  0.13354290 -0.03635186 -0.25198143
0.00861548  0.03685728 -0.43107049
   15    0.08035404 -0.01794252  0.00593441  0.07107057 -0.05162983
0.13725913 -0.08772329 -0.01746239
   16    0.25986800 -0.04468802 -0.08511587  0.06477731 -0.11200528
0.25817340 -0.25921797 -0.34104783
   17   -0.06717856 -0.00469603  0.07056925  0.09671474  0.03611732
-0.01007770  0.03409966  0.33165377
   18   -0.27180472  0.03657118  0.09648220 -0.19455841 -0.08258102
-0.29470433  0.25319682 -0.25200430
   19   -0.01359063  0.00251290 -0.05784283 -0.07594698 -0.05527643
-0.06573225  0.09526341 -0.24516735
   20    0.02024444  0.00888157 -0.08138302 -0.05177463 -0.04194692
-0.06596657  0.04850173 -0.21966168
   21   -0.00389504 -0.00984873  0.02491135  0.06040349 -0.12082035
-0.02053510 -0.03733465 -0.09949138
   22   -0.00694586 -0.00876229  0.02206760  0.03490797 -0.07921335
-0.00019795 -0.01759914 -0.07298368
   23    0.03576761  0.02629900 -0.08255786 -0.09934194  0.23771356
0.00416281  0.04315922  0.20943964
   24    0.17548409  0.06477669 -0.28720308 -0.16034905  0.31269073
-0.03404460  0.00656032  0.01409805

              9          10          11          12          13
14          15          16

           611.6665    626.4410    637.7587    738.1608    770.0733
780.6349    793.6659    887.7082
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    1   -0.00591192 -0.03362199 -0.58742939 -0.01699647  0.02320648
0.10523289 -0.18198620  0.09100951
    2   -0.10292660  0.02062510 -0.01216903  0.19141776 -0.58275500
0.10948594  0.07171033  0.19004456
    3    0.00129974 -0.08895815 -0.03570562  0.00018663 -0.06439734
-0.37247541  0.20307382  0.00617144
    4   -0.01189682 -0.11365879  0.70828632 -0.03072380  0.02462078
0.05028103 -0.12179614  0.20157502
    5   -0.06822762  0.02618505 -0.00310609  0.11580191 -0.41188605
0.06736302  0.01763049 -0.23688097
    6    0.02988454 -0.01955098 -0.04394745 -0.03835207 -0.05308284
-0.21284058  0.11309829  0.01454750
    7   -0.09110680 -0.37871762  0.02962398 -0.12591167 -0.00694839
-0.14881336 -0.10241605  0.28814893
    8    0.05764886  0.01187293  0.00222434  0.15070641 -0.54693186
0.10362614  0.05680629  0.05554514
    9    0.02466460 -0.10347343 -0.10341395  0.02413507 -0.04835027
-0.21082004  0.21450807 -0.08921032
   10    0.01221573 -0.15053655  0.14103738  0.04902928 -0.13361892
-0.02685525 -0.17158697 -0.79915952
   11   -0.04066341  0.02387707  0.03391639  0.03248628 -0.19298813
0.05017470  0.05856516  0.32626289
```

```
   12   -0.17184212 -0.61108561  0.04550923 -0.01546065 -0.12054414
-0.37701075 -0.20518910  0.02629499
   13    0.14824930  0.16197562  0.01794170 -0.45633636 -0.19825426
-0.05880730 -0.21461067  0.04120539
   14   -0.44052824 -0.13003248 -0.17814158  0.12647679  0.11918199
-0.10876194  0.22016194 -0.03621849
   15   -0.03463510 -0.07062919 -0.01733776  0.14370313  0.06597525
0.01072425  0.07925520 -0.01220263
   16   -0.09133562  0.06495832 -0.15400539 -0.44152933 -0.15600272
-0.10210865 -0.37967510 -0.01500486
   17    0.23321545  0.09506977  0.13721612  0.21454140  0.08064128
-0.14427519  0.21067730  0.00347520
   18   -0.27202661 -0.14601459 -0.08610463  0.09713975  0.00245238
0.12629741  0.16392373  0.01330604
   19    0.24593966  0.06108279 -0.08961940  0.52526757  0.03848070
-0.24217534 -0.47599793  0.10527162
   20    0.33684838 -0.17841047 -0.09386273  0.26545405  0.05205733
0.05539277 -0.23772259  0.05590941
   21    0.33230025 -0.28063445 -0.05836035 -0.19541314  0.01673145
0.17787456  0.21867428 -0.02955796
   22    0.18199719 -0.10386840 -0.03735131 -0.04865703 -0.02791316
0.00267277  0.09125750  0.00020154
   23   -0.51579528  0.25980549  0.10555440  0.14003573  0.10111532
0.03720158 -0.28383442 -0.00446100
   24   -0.05097221 -0.38768142 -0.01008874  0.05060304  0.08547115
0.63701369 -0.14780110 -0.00791986

             17          18          19          20          21
22          23          24

           984.8770   1305.8278   1313.6097   3002.4845   3005.7998
3098.2402   3106.0081   3669.6822
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    1    0.22244072 -0.00412849 -0.00934332 -0.00064790  0.00163794
-0.00020073 -0.00026787 -0.00024179
    2   -0.02383281 -0.05155956  0.02845684  0.00356323  0.00093033
0.00038414  0.00009614  0.00179139
    3    0.53042708  0.02851481  0.04792027  0.00055067 -0.00203795
-0.00051453 -0.00105294  0.00028256
    4    0.14501014 -0.00582876 -0.00684446 -0.00028418  0.00212270
0.00003028 -0.00006451  0.10857161
    5   -0.00641581 -0.03250913  0.01805477  0.00183158  0.00031709
-0.00074345  0.00071196  0.35445908
    6    0.32794496  0.01724987  0.03324627  0.00097138 -0.00176196
-0.00030457 -0.00021235 -0.00436110
    7   -0.27210665  0.00020599 -0.00242788  0.00075129 -0.00076015
-0.00199336 -0.00274231  0.08261107
    8    0.02862189 -0.06108848  0.03503659  0.00557595  0.00121036
0.00044209  0.00027037  0.12219599
    9   -0.67025773  0.01330613  0.02231088  0.00122030 -0.00563073
-0.00054347 -0.00146292 -0.02138515
   10    0.03613423  0.00206908 -0.00715323 -0.00042021  0.00063554
-0.00104582 -0.00051017 -0.37745815
   11   -0.00686310 -0.02478857  0.01412493  0.00134556  0.00157407
0.00046349  0.00013629 -0.83531446
   12    0.04051398  0.00436564  0.00972403  0.00021349 -0.00086518
-0.00346106 -0.00468164  0.01032206
   13   -0.02958828 -0.33444148 -0.07966459 -0.11767975 -0.17235514
-0.01388911  0.14601409 -0.00076137
   14    0.02843636 -0.60235930 -0.11823702  0.03841826  0.05321880
```

```
0.00952237 -0.07301534 -0.00004498
   15    0.01351946 -0.01996996 -0.00142733 -0.43596021 -0.63176765
-0.07499711  0.57025583 -0.00042666
   16   -0.02424690  0.05102292  0.02254724  0.15521974  0.24200173
-0.05916882  0.39509083  0.00050048
   17   -0.01190915 -0.30750190 -0.05621317  0.26075728  0.40039715
-0.08162121  0.57942682 -0.00008953
   18    0.01860994  0.56883515  0.11156354  0.10720972  0.16695579
-0.04548574  0.35122726 -0.00021163
   19   -0.04271527  0.01787024 -0.03624877 -0.28674503  0.19406247
0.37915291  0.03313841  0.00023306
   20    0.00236781 -0.09915325  0.23878544  0.43075027 -0.26273590
-0.56371927 -0.06551057 -0.00089465
   21    0.02331071 -0.16582459  0.70306721 -0.21022247  0.15705933
0.25774962  0.01683823 -0.00016363
   22    0.01179026  0.04260386 -0.17024050  0.57668117 -0.38487558
0.64099992  0.08344005 -0.00057111
   23   -0.02523210 -0.14822411  0.54436066  0.21229935 -0.13184229
0.18822145  0.07608943  0.00047825
   24    0.08239664 -0.18254204 -0.28082454 -0.03722384  0.15700869
0.08695771  0.12043803  0.00093786


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

                Frequency       Dipole Strength        Absorption
Intensity (degeneracy not counted)
                  cm-1           1e-40 esu2 cm2          km/mole
               ----------          ----------         ----------
               201.495490          142.401412           7.192133
               209.989111           15.632280           0.822805
               237.231767           24.649234           1.465731
               240.827362           38.681897           2.335026
               247.038126           81.873563           5.069741
               311.791802          270.465804          21.137573
               449.595122          581.514040          65.532972
               566.252107           17.845992           2.532962
               611.666549           20.117334           3.084347
               626.441025           27.378078           4.298938
               637.758675          659.699396         105.458243
               738.160808          139.671022          25.842550
               770.073268          139.866272          26.997473
               780.634911           66.627083          13.036975
               793.665870          399.028823          79.381635
               887.708189          293.093625          65.216077
               984.877009          437.644042         108.039133
              1305.827830           19.072135           6.242568
              1313.609726           23.287115           7.667612
              3002.484534            3.302467           2.485406
              3005.799848            4.332897           3.264499
              3098.240216            0.537018           0.417044
              3106.008145            0.937902           0.730194
              3669.682216           99.086345          91.142374


  Zero-Point Energy :      0.063326 a.u.
  ==================       1.723186 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)


                       201.495                     209.989
237.232
               ------------------------    ------------------------
------------------------
     1.Re         0.017  -0.027  -0.006        0.008   0.004   0.043
-0.028  -0.017   0.021
     2.O          0.014   0.160  -0.041       -0.003  -0.022  -0.397
-0.032   0.208  -0.049
     3.H         -0.057   0.195   0.399        0.015  -0.031  -0.543
-0.204   0.278   0.134
     4.O         -0.050   0.106   0.027        0.255  -0.006  -0.058
0.143  -0.064  -0.054
     5.C         -0.163   0.066   0.065       -0.170   0.022  -0.001
-0.032  -0.099  -0.107
     6.H          0.186   0.157   0.007       -0.472   0.024   0.061
-0.104  -0.287  -0.117
     7.H         -0.531   0.129   0.349        0.011  -0.002  -0.151
0.058  -0.046  -0.304
     8.C          0.000  -0.033   0.001       -0.215  -0.042  -0.004
0.277   0.135  -0.044
     9.H          0.237   0.018  -0.174       -0.195  -0.038  -0.018
0.468   0.243  -0.047
    10.H         -0.389  -0.035   0.042       -0.321  -0.080   0.012
0.393   0.164  -0.055


                       240.827                     247.038
311.792
               ------------------------    ------------------------
------------------------
     1.Re         0.024   0.017  -0.009        0.019   0.000   0.021
0.005  -0.019  -0.003
     2.O          0.031   0.067   0.024        0.021  -0.022  -0.017
0.012   0.073   0.051
     3.H         -0.005   0.083   0.053        0.052  -0.034   0.016
-0.086   0.101  -0.537
     4.O         -0.116  -0.239   0.044       -0.135   0.018   0.096
-0.032   0.136   0.019
     5.C         -0.200   0.047  -0.058       -0.027  -0.095  -0.159
-0.038   0.008   0.070
     6.H         -0.541  -0.156  -0.018       -0.059  -0.377  -0.188
-0.514   0.059   0.171
     7.H         -0.211   0.208  -0.340       -0.094   0.070  -0.386
0.181  -0.039  -0.088
     8.C          0.005  -0.067   0.099       -0.078   0.106  -0.170
0.002  -0.003  -0.068
     9.H         -0.225  -0.060   0.378       -0.065  -0.052  -0.504
-0.283  -0.108   0.056
    10.H          0.247  -0.255   0.084       -0.292   0.412  -0.161
0.448   0.076  -0.120
```

	449.595			566.252			611.667		
1.Re	-0.001	-0.001	0.000	-0.005	0.000	0.004	0.000	0.004	0.000
2.O	0.011	-0.022	-0.059	0.101	0.004	0.003	0.002	0.001	-0.005
3.H	-0.005	0.004	0.846	0.069	0.017	-0.022	-0.042	0.021	0.044
4.O	-0.005	0.031	0.004	-0.045	-0.008	0.022	0.011	-0.027	0.001
5.C	0.018	0.004	0.049	-0.029	0.003	-0.069	-0.039	-0.040	-0.083
6.H	-0.257	-0.009	0.102	-0.221	0.462	0.029	-0.033	0.463	-0.019
7.H	0.266	-0.058	-0.106	0.459	-0.362	0.079	-0.005	-0.279	0.324
8.C	-0.007	0.005	-0.043	-0.006	-0.005	-0.036	0.035	-0.021	0.080
9.H	-0.237	-0.073	0.070	0.414	0.260	0.021	-0.260	-0.361	-0.274
10.H	0.204	-0.003	-0.064	-0.213	-0.281	0.000	0.138	0.533	0.040

	626.441			637.759			738.161		
1.Re	-0.001	0.001	-0.004	0.050	0.001	0.003	-0.001	0.008	0.000
2.O	-0.024	0.003	0.008	-0.511	-0.001	0.007	-0.005	-0.001	-0.007
3.H	-0.018	-0.001	-0.017	-0.293	-0.093	0.061	0.111	-0.046	0.081
4.O	-0.019	-0.002	-0.032	-0.045	-0.005	0.030	-0.001	-0.008	-0.001
5.C	0.027	0.084	0.066	-0.031	-0.006	-0.064	0.102	-0.089	-0.002
6.H	-0.289	-0.180	0.094	-0.150	0.403	0.011	-0.464	0.121	0.143
7.H	0.338	0.130	-0.356	0.364	-0.320	0.095	-0.499	0.170	0.165
8.C	0.048	-0.103	0.081	-0.017	0.003	-0.053	-0.078	-0.071	-0.007
9.H	0.352	-0.195	-0.461	0.240	0.220	0.099	0.472	0.194	-0.103
10.H	-0.326	0.306	0.098	-0.057	-0.278	-0.035	0.322	0.119	-0.062

	770.073			780.635			793.666		
1.Re	-0.001	0.037	0.004	-0.006	-0.006	0.021	0.008	-0.003	-0.009
2.O	-0.005	0.012	0.004	0.002	0.000	-0.004			

```
0.007   0.005   0.001
     3.H          0.256  -0.094  -0.056         0.010  -0.003   0.037
0.102  -0.031   0.032
     4.O          0.001  -0.018  -0.004         0.008   0.002  -0.006
-0.013   0.001  -0.009
     5.C         -0.130  -0.199   0.120         0.007   0.234  -0.136
-0.108  -0.024   0.062
     6.H          0.318  -0.377   0.015         0.451   0.206  -0.242
0.350  -0.254  -0.056
     7.H          0.110  -0.395   0.201         0.038   0.247  -0.167
0.318  -0.225  -0.037
     8.C          0.086  -0.241  -0.161        -0.035  -0.171  -0.115
-0.146   0.049   0.094
     9.H          0.064  -0.315  -0.259         0.142  -0.085  -0.121
0.347   0.307   0.033
    10.H          0.106  -0.308  -0.170         0.633  -0.011  -0.206
0.459   0.411   0.015


                       887.708                     984.877
1305.828
               ------------------------    ------------------------
------------------------
     1.Re         0.003   0.007   0.000         0.031  -0.003   0.075
0.000  -0.002   0.001
     2.O          0.035  -0.060   0.000         0.026   0.005  -0.011
-0.001   0.000   0.000
     3.H         -0.929   0.332  -0.002         0.103  -0.020   0.000
0.003  -0.001   0.000
     4.O         -0.007  -0.004  -0.005        -0.368   0.031  -0.844
-0.001  -0.001  -0.001
     5.C         -0.008  -0.024   0.014        -0.006  -0.061  -0.025
0.028   0.107  -0.065
     6.H          0.042  -0.055   0.003        -0.002   0.116   0.001
-0.274  -0.620  -0.063
     7.H         -0.028  -0.023   0.032        -0.161  -0.052   0.108
0.028  -0.303   0.618
     8.C         -0.018  -0.027  -0.011        -0.004   0.070  -0.014
-0.008   0.020   0.014
     9.H          0.096   0.028  -0.032        -0.220   0.011   0.102
0.012  -0.051  -0.137
    10.H          0.033  -0.018  -0.019         0.018  -0.108  -0.002
0.058  -0.137   0.006


                      1313.610                    3002.485
3005.800
               ------------------------    ------------------------
------------------------
     1.Re         0.000  -0.001  -0.002         0.000   0.000   0.000
0.000   0.000   0.000
     2.O          0.000   0.000  -0.001         0.000   0.000   0.000
0.000   0.000   0.000
     3.H          0.002   0.000   0.006         0.000   0.000   0.001
0.000  -0.001   0.000
     4.O          0.002  -0.001   0.003         0.000   0.000   0.000
0.000   0.000   0.001
     5.C         -0.005  -0.024   0.015         0.005   0.025  -0.024
0.009   0.040  -0.034
     6.H          0.062   0.128   0.014         0.093  -0.041   0.434
0.138  -0.057   0.629
```

```
     7.H         -0.013   0.068  -0.129        -0.153  -0.253  -0.157
-0.237  -0.390  -0.241
     8.C         -0.036   0.098   0.071        -0.014   0.038   0.033
0.010  -0.026  -0.022
     9.H          0.032  -0.254  -0.643         0.246  -0.426   0.238
-0.170   0.290  -0.162
    10.H          0.298  -0.610   0.038        -0.078  -0.008  -0.617
0.053   0.004   0.411


                     3098.240                    3106.008
3669.682
               ------------------------    ------------------------
------------------------
     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
0.024   0.058  -0.001
     3.H          0.000   0.000   0.000         0.000   0.000   0.000
-0.375  -0.925   0.019
     4.O          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     5.C          0.006   0.007   0.010         0.040   0.045   0.076
0.000   0.000   0.000
     6.H         -0.014   0.010  -0.076        -0.116   0.079  -0.586
0.000   0.000   0.000
     7.H         -0.052  -0.086  -0.046        -0.358  -0.609  -0.332
0.000   0.000   0.000
     8.C         -0.034   0.047  -0.078         0.004  -0.006   0.011
0.000   0.000   0.000
     9.H          0.339  -0.592   0.291        -0.040   0.073  -0.036
-0.001  -0.001   0.000
    10.H          0.068   0.035   0.645        -0.012  -0.006  -0.099
0.001   0.001   0.000
```

List of All Frequencies:

Intensities
==========

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
201.495490	142.401412	7.192133
209.989111	15.632280	0.822805
237.231767	24.649234	1.465731
240.827362	38.681897	2.335026
247.038126	81.873563	5.069741
311.791802	270.465804	21.137573
449.595122	581.514040	65.532972
566.252107	17.845992	2.532962
611.666549	20.117334	3.084347
626.441025	27.378078	4.298938
637.758675	659.699396	105.458243
738.160808	139.671022	25.842550
770.073268	139.866272	26.997473

```
               780.634911           66.627083           13.036975
               793.665870          399.028823           79.381635
               887.708189          293.093625           65.216077
               984.877009          437.644042          108.039133
              1305.827830           19.072135            6.242568
              1313.609726           23.287115            7.667612
              3002.484534            3.302467            2.485406
              3005.799848            4.332897            3.264499
              3098.240216            0.537018            0.417044
              3106.008145            0.937902            0.730194
              3669.682216           99.086345           91.142374


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

  Pressure:                  1.000000 atm.
  Temperature:             298.150000 K


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

          519.8501        544.3715        557.6067
  ------------------------------------------------
            0.9362          0.0760         -0.3431
           -0.0872          0.9960         -0.0173
            0.3404          0.0461          0.9391


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

      298.15   Entropy (cal/mole-K):
42.425    26.559    14.654    83.638
               Internal Energy (Kcal/mole):
0.889     0.889    42.470    44.248
               Constant Volume Heat Capacity (cal/mole-K):
2.981     2.981    20.049    26.010

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