ReO2(CD3)3

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

Coordinates (Cartesian)
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Atom	bohr			angstrom	Geometric Variables				
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Re	1.672824	0.000000	0.000000	0.885220	0.000000	0.000000	1	2	3
2 O	3.349267	2.783318	0.000000	1.772355	1.472868	0.000000	4	5	6
3 O	3.151133	-2.896472	0.000000	1.667508	-1.532746	0.000000	7	8	9
4 C	-2.489014	0.081296	0.000000	-1.317129	0.043020	0.000000	10	11	12
5 H	-3.305568	0.951089	1.690243	-1.749231	0.503295	0.894438	13	14	15
6 H	-3.305568	0.951089	-1.690243	-1.749231	0.503295	-0.894438	16	17	18
7 H	-3.019126	-1.932462	0.000000	-1.597652	-1.022614	0.000000	19	20	21
8 C	0.564464	0.004882	-3.888607	0.298701	0.002583	-2.057762	22	23	24
9 H	2.396416	-0.251498	-4.847558	1.268128	-0.133087	-2.565217	25	26	27
10 H	-0.719052	-1.542643	-4.372191	-0.380506	-0.816331	-2.313663	28	29	30
11 H	-0.268803	1.820329	-4.425020	-0.142244	0.963276	-2.341619	31	32	33
12 C	0.564464	0.004882	3.888607	0.298701	0.002583	2.057762	34	35	36
13 H	-0.719052	-1.542643	4.372191	-0.380506	-0.816331	2.313663	37	38	39
14 H	2.396416	-0.251498	4.847558	1.268128	-0.133087	2.565217	40	41	42
15 H	-0.268803	1.820329	4.425020	-0.142244	0.963276	2.341619	43	44	45

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

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     9. H               2.00000000
    10. H               2.00000000
    11. H               2.00000000
    12. C              12.00000000
    13. H               2.00000000
    14. H               2.00000000
    15. H               2.00000000


AA

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

              1           2           3           4           5
6           7           8

            67.1256    181.9209    205.8878    235.6110    285.1536
420.9760    469.2646    564.0522
         ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1   -0.03890576 -0.03847802 -0.17663075 -0.39241723 -0.58100750
-0.20366955 -0.45921600  0.18001504
    2   -0.21979325  0.11009585 -0.60117783  0.30978645  0.01333026
-0.04710421 -0.03995357 -0.16086304
    3    0.18609324  0.14370741 -0.61563472 -0.24663101  0.34412275
-0.12627798 -0.16006265 -0.05015898
    4   -0.30862833 -0.06285854  0.02110689  0.27794811 -0.55357925
-0.04037996 -0.07187345 -0.08535644
    5   -0.34414763 -0.25146465  0.20880428 -0.54262772  0.28423448
-0.08079195 -0.09679608  0.15908037
    6   -0.74076201 -0.23533519 -0.05461317  0.06646766  0.23418896
-0.02005724  0.00237421 -0.19779342
    7   -0.02970744 -0.03832642 -0.15139931 -0.26390828 -0.18735743
0.47690493  0.33464574 -0.19166981
    8   -0.18731372  0.37201216 -0.03123619 -0.02232291  0.00129984  0.09997836
0.18065804  0.49672032
    9   -0.00472309 -0.01457352 -0.07808359 -0.18403818 -0.13135971
-0.53040507  0.51488991 -0.08200055
   10    0.00064919  0.01071580  0.01271103 -0.01237390  0.07346674
-0.12117354 -0.21088056  0.01815850
   11    0.00388462 -0.19390369 -0.09545353  0.07404300 -0.00255544
-0.02192596 -0.03151282  0.06002592
   12    0.00008236 -0.00265505 -0.00148715  0.00990230  0.00209963
0.00735662  0.00953109  0.04342981
   13    0.00123580  0.07983751  0.00683520 -0.25150020 -0.12513338
0.26847403  0.04982040 -0.52640681
   14   -0.17506428  0.47212978  0.07544121 -0.11038974 -0.02667551
0.04753320  0.01994688 -0.04208667
   15   -0.02302822 -0.25768091 -0.27251314 -0.05586170 -0.10817913
0.35337198  0.32723307  0.46666103
   16   -0.21788036  0.60593650  0.11445925 -0.10495605 -0.00122588
0.01032072  0.00765957  0.01164136
   17    0.00295397  0.01881728  0.06497876  0.15869481 -0.01834643
-0.39263977  0.34173753  0.05462535
   18    0.00465433  0.00212146  0.02129178  0.03950630  0.00886554
-0.03348928  0.02461084  0.00370969
   19    0.02620357 -0.00529299  0.02759178 -0.01105855  0.00226353
-0.00210541  0.00480680 -0.04977817
   20   -0.14035924  0.00101487 -0.20498804 -0.16446556 -0.09790154
-0.14507013  0.14680084  0.05915754
```

```
   21   -0.00370634 -0.00131666 -0.00633860 -0.01022434  0.00590313
0.01313198 -0.01469334 -0.00139680
   22    0.13431214 -0.04642113  0.03852416 -0.24444164 -0.07659126
-0.14827834  0.20705643 -0.25634970

              9          10          11          12          13
14          15          16

           569.9179    635.9824    912.3411    938.6632    953.6128
989.5878   1013.4789   1019.7903
         ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1    0.07219108  0.19300821  0.00504625  0.04064055 -0.00662938
-0.37501786  0.00684658  0.05666865
    2    0.11670700  0.00843983 -0.02762887 -0.07806139 -0.65552420
-0.02467210  0.00363644 -0.02689198
    3    0.06985285  0.18048636  0.05249706 -0.01354100  0.45034625
0.31315644 -0.00984533 -0.02347324
    4    0.09379000  0.00106286  0.04397554 -0.05440481  0.21993297
0.65787786 -0.01225551 -0.07705410
    5   -0.00885167  0.16298463  0.01584765 -0.13254286 -0.39298910
0.39319665 -0.00033362 -0.06861246
    6    0.13877045 -0.00362737 -0.00066917  0.09853816  0.36947000
-0.35342531 -0.01053932  0.05747305
    7   -0.07145091  0.21318759  0.39514582  0.42852868 -0.07987212
0.02209454  0.02989440  0.03664976
    8    0.20224636 -0.06902760  0.09756358  0.13898182  0.03579119
0.01695345  0.00766707 -0.14305411
    9   -0.03455557 -0.04433740 -0.44578821  0.36046397 -0.02295460
0.03946672 -0.01069997 -0.08241215
   10    0.01130352 -0.38630776  0.07133834  0.35409426 -0.06633108
0.13921995  0.02966472  0.43364129
   11   -0.37966626  0.00612388  0.04809909  0.04895806  0.00490434
0.00289533 -0.51850979 -0.02095943
   12    0.00978107 -0.00956174 -0.09853541 -0.09030718  0.04327810
-0.00293361 -0.01985908 -0.20578198
   13   -0.16327921  0.06410959 -0.28950770 -0.22987971  0.01788134
0.01285339  0.01262535  0.05062331
   14   -0.05566182  0.01812326 -0.26511457 -0.33134708  0.03511891
-0.03190848 -0.10457264  0.24354624
   15    0.13407631 -0.06478830 -0.28832882 -0.25746540  0.08070273
-0.00227344 -0.03294186  0.21670946
   16   -0.05177235  0.00360729  0.10572961  0.12512756 -0.00735235
0.01195741 -0.12248676 -0.03786890
   17   -0.07927882  0.53698010  0.32074166 -0.23807887  0.01639029
-0.06614180  0.02768084  0.21849134
   18    0.00467951  0.07034779  0.17281717 -0.11608989 -0.00783448
0.05700036  0.17204227  0.54313903
   19    0.13650934  0.02046095 -0.03829837 -0.01939153  0.01157511
-0.02095293  0.72905474 -0.17384377
   20   -0.56388238 -0.51397277  0.29986415 -0.26898557  0.05960104
-0.04015747  0.24853373 -0.05239427
   21   -0.00851883 -0.02103069 -0.21195132  0.20312591 -0.03006573
0.11789441  0.09728073  0.48469797
   22    0.60265298 -0.36743216  0.30872247 -0.25354162 -0.02426240
-0.04160746 -0.26093429  0.03499491

             17          18          19          20          21          22

          1058.0977   2115.3457   2123.9297   2250.5754   2265.5747   2298.1628
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1	-0.03722468	0.00095278	-0.00025116	-0.00311846	0.00132199	0.00090426
2	-0.02657480	0.00032244	-0.00080000	0.00176237	0.00083715	-0.00107167
3	0.02109969	0.00133775	0.00136075	-0.00036996	0.00334574	0.00105196
4	0.04005873	0.00191434	-0.00079670	-0.00132257	-0.00106398	-0.00017304
5	0.00791679	0.00118418	0.00213870	0.00021421	0.00310010	-0.00015881
6	-0.01707285	-0.00143496	-0.00131292	-0.00201674	0.00145117	0.00005033
7	0.16701010	0.02800821	-0.24166353	0.08455245	-0.01162637	0.00384796
8	-0.34385162	0.01759510	-0.11669535	-0.54840042	0.07682258	-0.01673306
9	0.04509330	-0.21322117	-0.02913392	0.00074260	0.01349348	0.00611713
10	-0.06385956	0.09593886	-0.11372101	-0.04467012	-0.63669948	-0.09248123
11	-0.09833505	-0.01177006	-0.03199249	-0.10596841	0.11607837	-0.69925334
12	-0.55332043	0.06865346	-0.58553169	0.52497441	-0.07407609	0.01933110
13	-0.45009419	0.01548001	0.18666866	-0.32570277	-0.22043627	0.00467538
14	0.46734792	0.06090530	-0.47223752	-0.04852826	-0.01364296	-0.14053684
15	0.05355344	-0.00492173	0.24011345	0.21905015	-0.23493244	-0.06612695
16	-0.09183980	-0.06854468	0.49072902	0.48691859	-0.04115725	-0.14851106
17	-0.10466808	0.31299794	0.04059414	-0.03733910	-0.27685968	-0.00240050
18	-0.22208115	-0.70771691	-0.08810135	0.02930179	0.24024478	-0.05828028
19	0.04651416	0.06911138	0.00997028	0.02139571	-0.02206450	-0.63615685
20	0.00606977	0.09383009	0.01322933	0.01049213	0.10424513	0.14653949
21	-0.17867607	0.55408052	0.06425371	0.08038582	0.55126612	0.01012382
22	-0.02703044	0.10624666	0.01355442	0.02175129	0.11884590	-0.16095956

Intensities
==========

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
67.125645	54.113894	0.910490
181.920898	4.662707	0.212617
205.887794	17.216713	0.888503
235.611008	22.631725	1.336569
285.153605	2.331025	0.166611
420.975956	0.428968	0.045265
469.264638	35.497168	4.175318
564.052157	9.174046	1.297055
569.917923	4.369843	0.624247
635.982445	19.273592	3.072457
912.341150	8.470349	1.937031
938.663222	23.678478	5.571109
953.612776	564.871749	135.020585
989.587762	218.313447	54.151797
1013.478916	39.992018	10.159354
1019.790325	4.615220	1.179727
1058.097727	5.312839	1.409063
2115.345698	2.643901	1.401860
2123.929731	8.604762	4.580966
2250.575418	7.662042	4.322313
2265.574683	14.226045	8.078684
2298.162813	2.676230	1.541638

AAA

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

1	2	3	4	5

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6           7           8

            88.5338    178.6491    203.8249    234.7384    338.0386
467.5008    565.5130    573.9012
          ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1   -0.09927140 -0.13028126  0.66909773  0.04768872 -0.32037027
-0.61745515 -0.13651513 -0.00954630
    2    0.09251122 -0.01745098 -0.48994934  0.75529746 -0.17112690
-0.36028764 -0.09823584 -0.09128370
    3   -0.09580516  0.20214568 -0.51975619 -0.61170534 -0.25235890
-0.47072932 -0.09057646  0.07262218
    4    0.03247278 -0.01566303  0.01717505 -0.01742981  0.53830380
-0.37323729  0.07193484 -0.00617873
    5   -0.08128655  0.00018812 -0.03012203  0.01222735 -0.27168525
0.11241910 -0.09133103  0.00683355
    6    0.06649268  0.00676796 -0.01310513  0.00417116  0.10868488
-0.16936366  0.55130858 -0.01444444
    7    0.19649004  0.02620796  0.01953131  0.05641346 -0.02923709
-0.00818256 -0.00408544  0.58435313
    8   -0.33090336 -0.11328116 -0.05237416  0.01939417  0.49919002
-0.19492297 -0.10279912  0.04180544
    9    0.09485670  0.00226529 -0.02521427 -0.01837025  0.22448170
0.06400028 -0.10664049 -0.01200311
   10    0.64270553  0.17446336  0.07615980 -0.06685999 -0.14198958
0.00593493 -0.03842005 -0.07458270
   11    0.57703043  0.13285085  0.05541957 -0.06961691  0.29582041
-0.19122588 -0.12101340 -0.05335102
   12   -0.01783768 -0.00515518 -0.00083712 -0.00418853  0.12999905
0.08286508 -0.76532186  0.11425445
   13    0.02395374 -0.08845239 -0.01609330 -0.01694895  0.00784059
0.01827856 -0.08762804  0.02256582
   14    0.15934434 -0.63697475 -0.11383220 -0.11706556 -0.04338461
-0.00755471  0.01498464  0.08109201
   15   -0.04280582  0.14459204  0.02594129  0.11824037  0.00439026
-0.01859639  0.11295404  0.77733300
   16    0.16882862 -0.66079353 -0.11899753 -0.10537449 -0.04491876
-0.01124221  0.02112780  0.09895154
   17   -0.02385949  0.09388619  0.00738664  0.01705391 -0.00291638
-0.01540002  0.03390386 -0.00788593

              9          10          11          12          13
14          15          16

           652.9975    914.3683   1009.1403   1021.5516   1028.5286
2116.5665   2261.5856   2283.2338
          ----------  ----------  ----------  ----------  ----------
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    1    0.14281782 -0.01026059 -0.00001928 -0.00627515 -0.00370155
-0.00280470 -0.00517769 -0.00027416
    2    0.04697843 -0.03341696  0.00688601 -0.01156267 -0.00379333
0.00270039 -0.00292708 -0.00002928
    3    0.07115876 -0.04140399 -0.00745552 -0.00245924  0.00419406
0.00380249 -0.00262485 -0.00010759
    4   -0.41952855 -0.02183013 -0.19133920 -0.13144013 -0.27794145
-0.00086923 -0.04415095  0.50296686
    5   -0.08741989  0.82196055 -0.10418393 -0.17434943 -0.04507115
-0.33176118 -0.05208811  0.23960157
    6    0.20536231  0.28810467  0.04839502  0.36681238 -0.14765209
0.02139094  0.59437535 -0.04849979
    7   -0.00654081 -0.00953625 -0.39337303  0.13410312  0.18855592
```

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-0.01405855 -0.10372565  0.04138795
    8    0.08917482  0.23803605 -0.12033437 -0.16803229 -0.00853324
-0.12968256 -0.11101196 -0.65746324
    9    0.85261402 -0.01580066 -0.13943839 -0.17727418 -0.17289414
-0.00661369 -0.11206505  0.31981249
   10   -0.08503914  0.01011084 -0.25384136 -0.25127192 -0.48209001
0.00894090  0.05108147 -0.37960386
   11    0.02999768  0.21552205  0.36217384  0.11258933  0.51898708
-0.11975671 -0.12690190 -0.00890218
   12   -0.05033221  0.09023441  0.05072247  0.25852812 -0.14985072
0.19927887  0.48264592  0.04319792
   13    0.00756526 -0.19404596  0.17398630  0.48111167 -0.37308179
-0.70461920 -0.21237333 -0.01952662
   14   -0.02027300  0.03047254  0.50515473 -0.32143831 -0.18450702
0.09990499  0.02141794  0.02741498
   15    0.01849042 -0.00466825  0.29118173 -0.15288871 -0.13003589
-0.00983303  0.02432054 -0.03137406
   16   -0.00032335  0.03534352 -0.41258469  0.26573099  0.14888310
0.07464432 -0.05921451 -0.03556650
   17    0.00957796  0.29396320  0.15093247  0.41051311 -0.31117489
0.55327774 -0.55231555 -0.03982009

            17

          2298.0166
          ----------
    1   -0.00069130
    2   -0.00170817
    3    0.00097579
    4   -0.03558699
    5   -0.02764512
    6    0.10360090
    7    0.62741626
    8    0.07905504
    9   -0.03428195
   10   -0.06986125
   11   -0.09398198
   12    0.00577973
   13    0.04312729
   14    0.35831979
   15   -0.46704334
   16   -0.47181045
   17    0.03770258


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

                Frequency       Dipole Strength        Absorption
Intensity (degeneracy not counted)
                  cm-1           1e-40 esu2 cm2          km/mole
               ----------          ----------         ----------
                88.533785            4.220458           0.093658
               178.649087            1.980847           0.088701
               203.824854          210.915290          10.775645
               234.738377            2.763278           0.162587
               338.038589            5.409358           0.458342
               467.500751          133.788910          15.677633
               565.513050          133.009998          18.854065
               573.901212            1.482407           0.213247
               652.997503            0.003857           0.000631
```

914.368289	0.629933	0.144375
1009.140348	1.490264	0.376958
1021.551598	0.131161	0.033585
1028.528589	5.622367	1.449485
2116.566541	0.799755	0.424294
2261.585646	2.758495	1.563736
2283.233822	15.475479	8.856713
2298.016614	0.023049	0.013277

Zero-Point Energy : 0.086141 a.u.
========== 2.344030 eV

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

	67.126			88.534			178.649		
1.Re	0.003	0.017	0.000	0.000	0.000	-0.006	0.000	0.000	0.008
2.O	-0.070	0.058	0.000	0.000	0.000	0.040	0.000	0.000	-0.014
3.O	0.085	0.056	0.000	0.000	0.000	-0.017	0.000	0.000	-0.075
4.C	0.006	0.203	0.000	0.000	0.000	0.022	0.000	0.000	0.000
5.H	0.068	0.263	0.000	0.084	0.473	-0.179	-0.012	-0.117	0.055
6.H	0.068	0.263	0.000	-0.084	-0.473	-0.179	0.012	0.117	0.055
7.H	-0.140	0.244	0.000	0.000	0.000	0.636	0.000	0.000	-0.146
8.C	-0.022	-0.233	0.002	0.023	0.023	-0.004	0.010	-0.022	0.002
9.H	-0.045	-0.375	-0.003	0.037	0.120	-0.005	0.066	0.332	0.015
10.H	-0.077	-0.231	0.137	0.099	-0.039	-0.014	0.327	-0.291	0.012
11.H	0.028	-0.250	-0.131	-0.072	-0.015	0.014	-0.350	-0.197	-0.017
12.C	-0.022	-0.233	-0.002	-0.023	-0.023	-0.004	-0.010	0.022	0.002
13.H	-0.077	-0.231	-0.137	-0.099	0.039	-0.014	-0.327	0.291	0.012
14.H	-0.045	-0.375	0.003	-0.037	-0.120	-0.005	-0.066	-0.332	0.015
15.H	0.028	-0.250	0.131	0.072	0.015	0.014	0.350	0.197	-0.017

	181.921			203.825			205.888		
1.Re	-0.002	0.006	0.000	0.000	0.000	0.090	0.016	0.053	0.000
2.O	0.051	-0.026	0.000	0.000	0.000	-0.543	0.268	-0.088	0.000
3.O	-0.067	-0.027	0.000	0.000	0.000	-0.481	-0.157	-0.024	0.000
4.C	-0.004	0.048	0.000	0.000	0.000	-0.057	-0.004	-0.178	0.000
5.H	0.000	0.055	-0.002	-0.095	0.122	-0.164	-0.130	-0.301	0.002
6.H	0.000	0.055	0.002	0.095	-0.122	-0.164	-0.130	-0.301	-0.002
7.H	-0.025	0.055	0.000	0.000	0.000	0.060	0.285	-0.257	0.000
8.C	0.019	-0.025	-0.004	0.123	0.020	0.009	-0.116	-0.102	0.035
9.H	0.080	0.334	0.014	0.142	-0.124	0.103	-0.193	-0.237	-0.072
10.H	0.344	-0.299	0.001	0.017	0.120	-0.009	-0.195	-0.097	0.226
11.H	-0.346	-0.205	-0.034	0.301	0.104	0.028	-0.106	-0.119	-0.042
12.C	0.019	-0.025	0.004	-0.123	-0.020	0.009	-0.116	-0.102	-0.035
13.H	0.344	-0.299	-0.001	-0.017	-0.120	-0.009	-0.195	-0.097	-0.226
14.H	0.080	0.334	-0.014	-0.142	0.124	0.103	-0.193	-0.237	0.072
15.H	-0.346	-0.205	0.034	-0.301	-0.104	0.028	-0.106	-0.119	0.042

	234.738			235.611			285.154		
1.Re	0.000	0.000	0.005	-0.031	0.024	0.000	0.086	-0.002	0.000
2.O	0.000	0.000	0.357	-0.014	0.021	0.000	-0.436	0.346	0.000
3.O	0.000	0.000	-0.388	-0.175	-0.046	0.000	-0.473	-0.320	0.000
4.C	0.000	0.000	-0.018	0.034	-0.074	0.000	0.144	-0.010	0.000
5.H	-0.020	0.014	-0.035	0.007	-0.115	0.010	0.161	0.000	-0.004
6.H	0.020	-0.014	-0.035	0.007	-0.115	-0.010	0.161	0.000	0.004
7.H	0.000	0.000	-0.005	0.133	-0.101	0.000	0.190	-0.015	0.000
8.C	-0.009	-0.181	-0.002	0.199	-0.064	-0.073	-0.112	0.005	0.096
9.H	-0.042	-0.421	0.001	0.303	-0.192	0.155	-0.141	0.005	0.033
10.H	-0.106	-0.159	0.181	0.194	-0.031	-0.160	-0.114	-0.015	0.176

```
    11.H          0.085  -0.192  -0.184         0.357  -0.038  -0.238
-0.133   0.003   0.138
    12.C          0.009   0.181  -0.002         0.199  -0.064   0.073
-0.112   0.005  -0.096
    13.H          0.106   0.159   0.181         0.194  -0.031   0.160
-0.114  -0.015  -0.176
    14.H          0.042   0.421   0.001         0.303  -0.192  -0.155
-0.141   0.005  -0.033
    15.H         -0.085   0.192  -0.184         0.357  -0.038   0.238
-0.133   0.003  -0.138


                       338.039                       420.976
467.501
               ------------------------      ------------------------
------------------------
     1.Re         0.000   0.000  -0.024        -0.017  -0.004   0.000
0.000   0.000  -0.053
     2.O          0.000   0.000   0.000        -0.016  -0.018   0.000
0.000   0.000  -0.012
     3.O          0.000   0.000  -0.014         0.012   0.013   0.000
0.000   0.000  -0.023
     4.C          0.000   0.000   0.303         0.300   0.047   0.000
0.000   0.000  -0.061
     5.H          0.142  -0.117   0.429         0.248  -0.032   0.007
0.019   0.001  -0.056
     6.H         -0.142   0.117   0.429         0.248  -0.032  -0.007
-0.019  -0.001  -0.056
     7.H          0.000   0.000   0.234         0.465   0.000   0.000
0.000   0.000  -0.066
     8.C          0.133  -0.013  -0.028        -0.042   0.008  -0.215
0.033  -0.005   0.311
     9.H          0.224  -0.052   0.151        -0.136   0.031  -0.390
0.112  -0.006   0.454
    10.H          0.164  -0.003  -0.141        -0.079   0.011  -0.144
0.070  -0.013   0.265
    11.H          0.225   0.001  -0.128        -0.118  -0.003  -0.147
0.088   0.010   0.302
    12.C         -0.133   0.013  -0.028        -0.042   0.008   0.215
-0.033   0.005   0.311
    13.H         -0.164   0.003  -0.141        -0.079   0.011   0.144
-0.070   0.013   0.265
    14.H         -0.224   0.052   0.151        -0.136   0.031   0.390
-0.112   0.006   0.454
    15.H         -0.225  -0.001  -0.128        -0.118  -0.003   0.147
-0.088  -0.010   0.302


                       469.265                       564.052
565.513
               ------------------------      ------------------------
------------------------
     1.Re        -0.038  -0.003   0.000        -0.012   0.011   0.000
0.000   0.000  -0.009
     2.O          0.016  -0.036   0.000         0.049   0.004   0.000
0.000   0.000  -0.008
     3.O          0.055   0.025   0.000        -0.037   0.031   0.000
0.000   0.000   0.002
     4.C          0.285   0.086   0.000         0.119  -0.194   0.000
0.000   0.000   0.050
     5.H          0.160  -0.061   0.010         0.441   0.159  -0.036
```

```
-0.032  -0.033   0.050
     6.H          0.160  -0.061  -0.010         0.441   0.159   0.036
0.032   0.033   0.050
     7.H          0.596   0.000   0.000        -0.625   0.010   0.000
0.000   0.000   0.020
     8.C          0.005  -0.002   0.214         0.012  -0.047   0.027
0.151   0.001   0.011
     9.H          0.077   0.015   0.348        -0.015   0.044  -0.045
-0.117  -0.007  -0.489
    10.H          0.048  -0.013   0.150        -0.033   0.016  -0.049
-0.012   0.022   0.389
    11.H          0.041   0.009   0.211         0.012   0.008   0.210
-0.036  -0.016   0.254
    12.C          0.005  -0.002  -0.214         0.012  -0.047  -0.027
-0.151  -0.001   0.011
    13.H          0.048  -0.013  -0.150        -0.033   0.016   0.049
0.012  -0.022   0.389
    14.H          0.077   0.015  -0.348        -0.015   0.044   0.045
0.117   0.007  -0.489
    15.H          0.041   0.009  -0.211         0.012   0.008  -0.210
0.036   0.016   0.254


                      569.918                     573.901
635.982
               ------------------------    ------------------------
------------------------
     1.Re         0.005   0.007   0.000         0.000   0.000   0.001
0.013   0.001   0.000
     2.O          0.016   0.015   0.000         0.000   0.000   0.026
0.031   0.013   0.000
     3.O         -0.024   0.005   0.000         0.000   0.000  -0.029
0.022  -0.009   0.000
     4.C         -0.041   0.061   0.000         0.000   0.000   0.001
0.028  -0.026   0.000
     5.H         -0.140  -0.039   0.008         0.013  -0.004   0.009
0.078   0.028  -0.008
     6.H         -0.140  -0.039  -0.008        -0.013   0.004   0.009
0.078   0.028   0.008
     7.H          0.180   0.003   0.000         0.000   0.000  -0.007
-0.058  -0.001   0.000
     8.C         -0.003  -0.129  -0.011         0.003  -0.138  -0.003
-0.170   0.001  -0.015
     9.H          0.006   0.128  -0.062        -0.001   0.132  -0.082
0.070   0.011   0.437
    10.H         -0.054   0.044  -0.439        -0.056   0.042  -0.433
-0.009  -0.016  -0.418
    11.H          0.059   0.039   0.469         0.053   0.034   0.510
0.009   0.006  -0.299
    12.C         -0.003  -0.129   0.011        -0.003   0.138  -0.003
-0.170   0.001   0.015
    13.H         -0.054   0.044   0.439         0.056  -0.042  -0.433
-0.009  -0.016   0.418
    14.H          0.006   0.128   0.062         0.001  -0.132  -0.082
0.070   0.011  -0.437
    15.H          0.059   0.039  -0.469        -0.053  -0.034   0.510
0.009   0.006   0.299


                      652.998                     912.341
914.368
```

1.Re	0.000	0.000	-0.009	0.000	-0.002	0.000	0.000	0.000	-0.001
2.O	0.000	0.000	0.009	0.016	0.024	0.000	0.000	0.000	-0.009
3.O	0.000	0.000	0.005	0.002	-0.001	0.000	0.000	0.000	-0.009
4.C	0.000	0.000	0.176	0.161	0.033	0.000	0.000	0.000	-0.005
5.H	-0.671	0.062	-0.160	-0.289	-0.181	-0.082	0.018	0.012	0.000
6.H	0.671	-0.062	-0.160	-0.289	-0.181	0.082	-0.018	-0.012	0.000
7.H	0.000	0.000	-0.061	-0.369	0.155	0.000	0.000	0.000	-0.013
8.C	-0.008	-0.001	0.007	-0.038	0.005	-0.151	0.042	-0.002	0.193
9.H	0.006	0.022	0.029	0.162	-0.037	0.267	-0.204	0.026	-0.311
10.H	0.012	-0.006	-0.037	-0.022	-0.121	0.250	0.022	0.169	-0.362
11.H	0.012	0.005	-0.015	-0.005	0.129	0.257	-0.019	-0.178	-0.360
12.C	0.008	0.001	0.007	-0.038	0.005	0.151	-0.042	0.002	0.193
13.H	-0.012	0.006	-0.037	-0.022	-0.121	-0.250	-0.022	-0.169	-0.362
14.H	-0.006	-0.022	0.029	0.162	-0.037	-0.267	0.204	-0.026	-0.311
15.H	-0.012	-0.005	-0.015	-0.005	0.129	-0.257	0.019	0.178	-0.360

	938.663			953.613			989.588		
1.Re	-0.003	0.005	0.000	0.001	0.103	0.000	-0.056	-0.004	0.000
2.O	0.014	0.005	0.000	-0.298	-0.534	0.000	0.346	0.540	0.000
3.O	0.041	-0.065	0.000	0.282	-0.600	0.000	0.279	-0.501	0.000
4.C	-0.189	-0.048	0.000	0.081	-0.048	0.000	0.028	0.014	0.000
5.H	0.326	0.243	0.076	-0.091	-0.031	-0.085	-0.071	-0.058	-0.005
6.H	0.326	0.243	-0.076	-0.091	-0.031	0.085	-0.071	-0.058	0.005
7.H	0.428	-0.193	0.000	-0.290	0.040	0.000	-0.105	0.042	0.000
8.C	-0.034	-0.004	-0.123	0.013	-0.021	0.018	0.069	0.000	0.029
9.H	0.126	0.013	0.199	-0.012	-0.025	-0.032	-0.008	-0.025	-0.119
10.H	-0.019	-0.116	0.225	-0.020	0.050	-0.117	-0.099	0.164	-0.073
11.H	0.033	0.119	0.212	-0.038	-0.032	0.048	-0.167	-0.131	-0.075
12.C	-0.034	-0.004	0.123	0.013	-0.021	-0.018			

```
0.069   0.000  -0.029
    13.H         -0.019  -0.116  -0.225        -0.020   0.050   0.117
-0.099   0.164   0.073
    14.H          0.126   0.013  -0.199        -0.012  -0.025   0.032
-0.008  -0.025   0.119
    15.H          0.033   0.119  -0.212        -0.038  -0.032  -0.048
-0.167  -0.131   0.075


                     1009.140                    1013.479
1019.790
               ------------------------    ------------------------
------------------------
     1.Re         0.000   0.000   0.000         0.000   0.000   0.000
-0.003   0.002   0.000
     2.O          0.000   0.000  -0.002        -0.004  -0.005   0.000
0.015   0.020   0.000
     3.O          0.000   0.000   0.002         0.000  -0.002   0.000
0.021  -0.036   0.000
     4.C          0.000   0.000   0.069         0.011   0.002   0.000
-0.013   0.045   0.000
     5.H          0.088   0.228  -0.011        -0.030  -0.004  -0.015
0.079  -0.177   0.153
     6.H         -0.088  -0.228  -0.011        -0.030  -0.004   0.015
0.079  -0.177  -0.153
     7.H          0.000   0.000  -0.387        -0.005   0.004   0.000
-0.097   0.061   0.000
     8.C         -0.003   0.080   0.002         0.002  -0.093  -0.003
-0.081  -0.005   0.025
     9.H         -0.088  -0.432  -0.025         0.099   0.507   0.020
-0.158   0.106  -0.162
    10.H          0.274  -0.107  -0.151        -0.312   0.117   0.183
0.255  -0.285   0.039
    11.H         -0.155   0.050   0.159         0.196  -0.054  -0.192
0.411   0.207  -0.026
    12.C          0.003  -0.080   0.002         0.002  -0.093   0.003
-0.081  -0.005  -0.025
    13.H         -0.274   0.107  -0.151        -0.312   0.117  -0.183
0.255  -0.285  -0.039
    14.H          0.088   0.432  -0.025         0.099   0.507  -0.020
-0.158   0.106   0.162
    15.H          0.155  -0.050   0.159         0.196  -0.054   0.192
0.411   0.207   0.026


                     1021.552                    1028.529
1058.098
               ------------------------    ------------------------
------------------------
     1.Re         0.000   0.000   0.000         0.000   0.000   0.000
0.002   0.002   0.000
     2.O          0.000   0.000  -0.002         0.000   0.000   0.001
-0.010  -0.018   0.000
     3.O          0.000   0.000   0.001         0.000   0.000  -0.002
-0.005   0.006   0.000
     4.C          0.000   0.000  -0.046         0.000   0.000   0.100
-0.066   0.107   0.000
     5.H         -0.084  -0.170   0.006         0.133   0.329  -0.015
0.267  -0.409   0.409
     6.H          0.084   0.170   0.006        -0.133  -0.329  -0.015
0.267  -0.409  -0.409
```

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     7.H          0.000   0.000   0.284         0.000   0.000  -0.558
-0.151   0.125   0.000
     8.C          0.076   0.028  -0.019         0.046  -0.039  -0.018
0.027  -0.002  -0.014
     9.H          0.120  -0.229   0.144         0.129   0.178   0.088
0.067  -0.025   0.077
    10.H         -0.163   0.243  -0.088        -0.273   0.196   0.075
-0.111   0.107  -0.004
    11.H         -0.442  -0.183   0.074        -0.119  -0.128  -0.066
-0.157  -0.075   0.020
    12.C         -0.076  -0.028  -0.019        -0.046   0.039  -0.018
0.027  -0.002   0.014
    13.H          0.163  -0.243  -0.088         0.273  -0.196   0.075
-0.111   0.107   0.004
    14.H         -0.120   0.229   0.144        -0.129  -0.178   0.088
0.067  -0.025  -0.077
    15.H          0.442   0.183   0.074         0.119   0.128  -0.066
-0.157  -0.075  -0.020


                     2115.346                    2116.567
2123.930
               ------------------------    ------------------------
------------------------
     1.Re         0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     2.O          0.000   0.001   0.000         0.000   0.000  -0.001
0.000   0.000   0.000
     3.O          0.000  -0.001   0.000         0.000   0.000  -0.001
-0.001   0.000   0.000
     4.C          0.010   0.005   0.000         0.000   0.000   0.000
0.089   0.035   0.000
     5.H         -0.020   0.026   0.050         0.002  -0.002  -0.003
-0.178   0.221   0.424
     6.H         -0.020   0.026  -0.050        -0.002   0.002  -0.003
-0.178   0.221  -0.424
     7.H         -0.021  -0.086   0.000         0.000   0.000  -0.001
-0.159  -0.656   0.000
     8.C          0.015  -0.003  -0.063        -0.015   0.003   0.063
-0.003   0.000   0.009
     9.H         -0.447   0.063   0.226         0.450  -0.064  -0.228
0.056  -0.008  -0.029
    10.H          0.213   0.258   0.068        -0.214  -0.259  -0.069
-0.025  -0.030  -0.010
    11.H          0.139  -0.303   0.077        -0.140   0.306  -0.078
-0.019   0.035  -0.010
    12.C          0.015  -0.003   0.063         0.015  -0.003   0.063
-0.003   0.000  -0.009
    13.H          0.213   0.258  -0.068         0.214   0.259  -0.069
-0.025  -0.030   0.010
    14.H         -0.447   0.063  -0.226        -0.450   0.064  -0.228
0.056  -0.008   0.029
    15.H          0.139  -0.303  -0.077         0.140  -0.306  -0.078
-0.019   0.035   0.010


                     2250.575                    2261.586
2265.575
               ------------------------    ------------------------
------------------------
     1.Re         0.000   0.000   0.000         0.000   0.000   0.000
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```
0.000   0.000   0.000
     2.O          0.000  -0.001   0.000         0.000   0.000   0.000
-0.001   0.000   0.000
     3.O          0.001  -0.001   0.000         0.000   0.000   0.000
-0.001   0.000   0.000
     4.C          0.033  -0.178   0.000         0.000   0.000   0.016
0.005  -0.025   0.000
     5.H         -0.179   0.196   0.401         0.019  -0.024  -0.047
-0.029   0.030   0.057
     6.H         -0.179   0.196  -0.401        -0.019   0.024  -0.047
-0.029   0.030  -0.057
     7.H          0.182   0.672   0.000         0.000   0.000   0.002
0.024   0.091   0.000
     8.C         -0.018   0.008   0.000        -0.129   0.022   0.005
0.130  -0.018  -0.004
     9.H          0.052  -0.007  -0.029         0.406  -0.057  -0.217
-0.405   0.058   0.212
    10.H          0.021   0.026   0.008         0.212   0.263   0.077
-0.219  -0.271  -0.080
    11.H          0.029  -0.063   0.017         0.150  -0.336   0.095
-0.143   0.322  -0.091
    12.C         -0.018   0.008   0.000         0.129  -0.022   0.005
0.130  -0.018   0.004
    13.H          0.021   0.026  -0.008        -0.212  -0.263   0.077
-0.219  -0.271   0.080
    14.H          0.052  -0.007   0.029        -0.406   0.057  -0.217
-0.405   0.058  -0.212
    15.H          0.029  -0.063  -0.017        -0.150   0.336   0.095
-0.143   0.322   0.091


                     2283.234                    2298.017
2298.163
               ------------------------     ------------------------
------------------------
     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.O          0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     4.C          0.000   0.000  -0.189         0.000   0.000   0.013
-0.001   0.005   0.000
     5.H         -0.258   0.294   0.569         0.018  -0.019  -0.040
0.007  -0.007  -0.015
     6.H          0.258  -0.294   0.569        -0.018   0.019  -0.040
0.007  -0.007   0.015
     7.H          0.000   0.000  -0.009         0.000   0.000  -0.002
-0.008  -0.027   0.000
     8.C         -0.012  -0.008   0.001        -0.021  -0.132   0.002
0.020   0.132  -0.002
     9.H          0.038  -0.006  -0.019         0.010  -0.004  -0.005
-0.004   0.004   0.002
    10.H          0.037   0.046   0.016         0.315   0.373   0.114
-0.311  -0.368  -0.112
    11.H         -0.001   0.003   0.001        -0.197   0.418  -0.121
0.200  -0.426   0.124
    12.C          0.012   0.008   0.001         0.021   0.132   0.002
0.020   0.132   0.002
    13.H         -0.037  -0.046   0.016        -0.315  -0.373   0.114
-0.311  -0.368   0.112
```

```
    14.H         -0.038   0.006  -0.019        -0.010   0.004  -0.005
-0.004   0.004  -0.002
    15.H          0.001  -0.003   0.001         0.197  -0.418  -0.121
0.200  -0.426  -0.124
```

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
67.125645	54.113894	0.910490
88.533785	4.220458	0.093658
178.649087	1.980847	0.088701
181.920898	4.662707	0.212617
203.824854	210.915290	10.775645
205.887794	17.216713	0.888503
234.738377	2.763278	0.162587
235.611008	22.631725	1.336569
285.153605	2.331025	0.166611
338.038589	5.409358	0.458342
420.975956	0.428968	0.045265
467.500751	133.788910	15.677633
469.264638	35.497168	4.175318
564.052157	9.174046	1.297055
565.513050	133.009998	18.854065
569.917923	4.369843	0.624247
573.901212	1.482407	0.213247
635.982445	19.273592	3.072457
652.997503	0.003857	0.000631
912.341150	8.470349	1.937031
914.368289	0.629933	0.144375
938.663222	23.678478	5.571109
953.612776	564.871749	135.020585
989.587762	218.313447	54.151797
1009.140348	1.490264	0.376958
1013.478916	39.992018	10.159354
1019.790325	4.615220	1.179727
1021.551598	0.131161	0.033585
1028.528589	5.622367	1.449485
1058.097727	5.312839	1.409063
2115.345698	2.643901	1.401860
2116.566541	0.799755	0.424294
2123.929731	8.604762	4.580966
2250.575418	7.662042	4.322313
2261.585646	2.758495	1.563736
2265.574683	14.226045	8.078684
2283.233822	15.475479	8.856713
2298.016614	0.023049	0.013277
2298.162813	2.676230	1.541638

==========

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

  Pressure:                  1.000000 atm.
  Temperature:             298.150000 K



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

         774.8990        915.4089       1105.7316
  ------------------------------------------------
           0.0000          1.0000         -0.0046
           0.0000          0.0046          1.0000
           1.0000          0.0000          0.0000


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

      298.15   Entropy (cal/mole-K):
42.711    28.152    29.429   100.293
               Internal Energy (Kcal/mole):
0.889     0.889    59.003    60.780
               Constant Volume Heat Capacity (cal/mole-K):
2.981     2.981    32.929    38.890

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