Supplementary Material (ESI) for Dalton Transactions

ReO2CD3CD2

```
                                          ***************************
                                          *  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        1.689724    0.000000    0.000000       0.894163
0.000000    0.000000      1       2       3
    2 O         3.144271    0.569278    2.856530       1.663876
0.301249    1.511610      4       5       6
    3 O         3.144271    0.569278   -2.856530       1.663876
0.301249   -1.511610      7       8       9
    4 C         0.156052   -3.229801    0.000000       0.082579
-1.709136    0.000000     10      11      12
    5 H        -0.180699   -4.278201    1.751561      -0.095622
-2.263926    0.926886     13      14      15
    6 H        -0.180699   -4.278201   -1.751561      -0.095622
-2.263926   -0.926886     16      17      18
    7 C        -1.535315    2.345550    0.000000      -0.812454
1.241211    0.000000     19      20      21
    8 H        -0.870744    4.315431    0.000000      -0.460778
2.283627    0.000000     22      23      24
    9 H        -2.683429    1.993333   -1.688484      -1.420009
1.054826   -0.893507     25      26      27
   10 H        -2.683429    1.993333    1.688484      -1.420009
1.054826    0.893507     28      29      30
  ---------------------------------------------------------------------------
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  Atomic Masses:
  --------------
     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. C              12.00000000
     8. H               2.00000000
     9. H               2.00000000
    10. H               2.00000000


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

=== AA ===

Symmetry Displacements

	1			2			3		
1.Re	0.037	0.000	0.000	0.000	0.037	0.000	0.000	0.000	0.000
2.O	-0.105	-0.002	0.000	0.003	-0.118	0.000	0.000	0.000	0.177
3.O	-0.105	-0.002	0.000	0.003	-0.118	0.000	0.000	0.000	-0.177
4.C	-0.110	0.002	0.000	-0.023	-0.098	0.000	0.000	0.000	0.000
5.H	-0.111	0.002	0.000	-0.030	-0.096	0.000	0.000	0.000	0.000
6.H	-0.111	0.002	0.000	-0.030	-0.096	0.000	0.000	0.000	0.000
7.C	-0.103	0.004	0.000	0.015	-0.087	0.000	0.000	0.000	0.000
8.H	-0.101	0.003	0.000	0.028	-0.091	0.000	0.000	0.000	0.000
9.H	-0.104	0.005	0.000	0.013	-0.079	0.000	0.000	0.000	0.000
10.H	-0.104	0.005	0.000	0.013	-0.079	0.000	0.000	0.000	0.000

	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	0.126	0.012	0.000	0.000	0.095	0.000	0.000	0.000	0.000
3.O	0.126	0.012	0.000	0.000	0.095	0.000	0.000	0.000	0.000
4.C	-0.101	-0.005	0.000	-0.103	-0.126	0.000	0.172	-0.050	0.000
5.H	-0.095	-0.007	0.000	-0.140	-0.114	0.000	-0.363	-0.034	0.000
6.H	-0.095	-0.007	0.000	-0.140	-0.114	0.000	-0.363	-0.034	0.000
7.C	-0.134	-0.015	0.000	0.095	-0.066	0.000	-0.041	0.032	0.000
8.H	-0.145	-0.011	0.000	0.164	-0.090	0.000	0.055	0.000	0.000
9.H	-0.132	-0.022	0.000	0.082	-0.026	0.000	-0.058	0.088	0.000
10.H	-0.132	-0.022	0.000	0.082	-0.026	0.000	-0.058	0.088	0.000

	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.O	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
4.C	0.000	0.220	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5.H	-0.136	-0.151	0.000	-0.058	0.046	0.000	0.015	-0.229	0.000
6.H	-0.136	-0.151	0.000	-0.058	0.046	0.000	0.015	-0.229	0.000
7.C	0.027	-0.118	0.000	0.176	-0.004	0.000	0.000	0.194	0.000
8.H	0.075	-0.134	0.000	-0.369	0.021	0.000	-0.016	-0.232	0.000
9.H	0.018	-0.089	0.000	-0.285	-0.045	0.000	-0.007	-0.238	0.000
10.H	0.018	-0.089	0.000	-0.285	-0.045	0.000	-0.007	-0.238	0.000

	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.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	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5.H	0.000	0.000	0.500	0.148	-0.234	0.000	0.000	0.293	0.000
6.H	0.000	0.000	-0.500	0.148	-0.234	0.000	0.000	0.293	0.000
7.C	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
8.H	0.000	0.000	0.000	0.220	-0.092	0.000	0.298	-0.428	0.000
9.H	0.000	0.000	0.000	-0.258	0.280	0.000	-0.149	-0.079	0.000
10.H	0.000	0.000	0.000	-0.258	0.280	0.000	-0.149	-0.079	0.000

	13			14		
1.Re	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
3.O	0.000	0.000	0.000	0.000	0.000	0.000
4.C	0.000	0.000	0.000	0.000	0.000	0.000
5.H	0.000	0.000	0.000	0.000	0.000	0.000
6.H	0.000	0.000	0.000	0.000	0.000	0.000

```
     7.C          0.000   0.000   0.000         0.000   0.000   0.000
     8.H          0.355   0.455   0.000         0.000   0.000   0.000
     9.H         -0.178  -0.228   0.000         0.000   0.000   0.500
    10.H         -0.178  -0.228   0.000         0.000   0.000  -0.500

  Largest computed component in inactive z Dipole derivative=  0.3361E-17
  (symmetry index=  1)
  Deviation may result from numerical integration and/or the non-linearity
  in the transformations between Cartesian and Z-matrix coordinates.


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

              1           2           3           4           5
6           7           8

           182.6575    210.5137    281.6502    490.8630    572.6299
647.1731    694.0383    933.4117
         ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1    0.40162204 -0.41664448 -0.46404707  0.47209861  0.01146907
-0.15239310  0.23947550 -0.01676881
    2    0.26336185  0.61465646 -0.29350402 -0.36377067 -0.07834824
0.05048871  0.52417633  0.02331611
    3    0.00974768 -0.07204251 -0.53518593  0.03130989 -0.00134529
-0.02929834  0.03657732 -0.03455270
    4    0.57332174  0.15528540  0.58062692  0.35686744 -0.09505741
-0.10836178  0.17443555 -0.06484478
    5   -0.07177369 -0.61336064  0.25879409 -0.43678599 -0.02816167
0.05876357  0.54705617  0.04442511
    6   -0.09419509 -0.01854088 -0.01903688  0.25836098 -0.47950238
0.76860041  0.16840025 -0.04007859
    7    0.40134758 -0.14238945 -0.04142488 -0.38820378 -0.18197592
-0.17738063 -0.12451201  0.02054317
    8    0.17366121 -0.01577600  0.00102038 -0.00067069  0.25058387
0.23012258 -0.08303713  0.72806917
    9   -0.12469188  0.05251323  0.03859340  0.09106701  0.43524256
0.03693765  0.22746884 -0.44263539
   10    0.00073677  0.00500047 -0.00946334  0.00031010 -0.03258366
0.02022460 -0.17566625  0.00926568
   11   -0.45304840  0.11772725  0.04477435  0.25810611 -0.38361499
-0.51911800  0.33032664  0.29291624
   12    0.11980726 -0.07445015 -0.04785904 -0.18004471 -0.56189838
-0.10582160 -0.30677116 -0.18299632
   13    0.00489530 -0.00217157  0.00207616 -0.02429366  0.05493633
0.01748983 -0.01267029 -0.20685439
   14    0.01029389  0.00570722  0.00563236  0.01748614  0.04078157
0.01566888 -0.01058384  0.31875000

              9          10          11          12          13          14

           983.7164   1016.6002   1030.6597   2123.1404   2197.4819   2262.2749
         ----------  ----------  ----------  ----------  ----------  ----------
    1    0.36880831 -0.04969710  0.08587947  0.00006564  0.00630333  0.00102034
    2    0.14618601 -0.01620368  0.16887069 -0.00063220  0.01476820 -0.00187808
    3   -0.83397252  0.09048891  0.01385313 -0.00196954  0.00491940  0.00042187
    4   -0.34624038  0.03723553  0.07684992 -0.00329576  0.00968703  0.00404454
    5   -0.10467877  0.01773144  0.20894080  0.00136034  0.02130025 -0.00259552
    6   -0.00422913 -0.04554199 -0.21911806 -0.00467573 -0.15134076 -0.00246792
    7    0.01046254 -0.05209930 -0.64147898  0.00030459 -0.41400851  0.00074747
```

```
    8   -0.06360535 -0.21836006  0.01960156  0.23298372  0.02150863 -0.45826612
    9   -0.04940312 -0.41127099 -0.17208144 -0.24679987 -0.20960864 -0.47686533
   10    0.00544118  0.03713582  0.55737023 -0.00504131 -0.80954273  0.00380747
   11   -0.03136464 -0.13126535 -0.14784869  0.11223115 -0.17530848 -0.13153673
   12   -0.00327513 -0.37330604  0.29964030 -0.13402664  0.27263975 -0.41161220
   13   -0.05771569 -0.57345633  0.04140825  0.70250482 -0.00232653  0.35452406
   14   -0.07273951 -0.52815332  0.02879783 -0.60055977  0.00588317  0.50012879


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

                Frequency       Dipole Strength        Absorption
Intensity (degeneracy not counted)
                  cm-1           1e-40 esu2 cm2          km/mole
               ----------          ----------         ----------
               182.657540           81.541441           3.733310
               210.513673           92.160118           4.862968
               281.650180           14.604869           1.031064
               490.863008           67.538693           8.309809
               572.629903           79.108350          11.354667
               647.173090           94.465219          15.323941
               694.038275           35.893367           6.244184
               933.411687            1.154451           0.270101
               983.716356          218.216902          53.806699
              1016.600163            5.915107           1.507269
              1030.659726           45.444263          11.740117
              2123.140397            0.623551           0.331840
              2197.481944           12.495525           6.882685
              2262.274902            2.059579           1.167890


                                        === AAA ===

  Symmetry Displacements


                          1                              2
3
               ------------------------      ------------------------
------------------------
     1.Re          0.000   0.000   0.037         0.000   0.000   0.000
0.000   0.000   0.000
     2.O           0.021  -0.003  -0.119         0.113   0.028   0.091
0.068  -0.056   0.000
     3.O          -0.021   0.003  -0.119        -0.113  -0.028   0.091
-0.068   0.056   0.000
     4.C           0.000   0.000  -0.101         0.000   0.000  -0.097
0.000   0.000   0.086
     5.H           0.013  -0.002  -0.099         0.069   0.017  -0.074
-0.242  -0.034   0.019
     6.H          -0.013   0.002  -0.099        -0.069  -0.017  -0.074
0.242   0.034   0.019
     7.C           0.000   0.000  -0.083         0.000   0.000  -0.086
0.000   0.000  -0.039
     8.H           0.000   0.000  -0.086         0.000   0.000  -0.132
0.000   0.000   0.092
     9.H          -0.012   0.002  -0.075        -0.067  -0.017  -0.037
0.233   0.033  -0.205
    10.H           0.012  -0.002  -0.075         0.067   0.017  -0.037
-0.233  -0.033  -0.205
```

	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	0.000	0.118	0.000	0.000	0.000	0.000	0.000	0.000	0.000
3.O	0.000	-0.118	0.000	0.000	0.000	0.000	0.000	0.000	0.000
4.C	0.000	0.000	-0.070	0.000	0.000	0.162	0.000	0.000	0.000
5.H	-0.134	-0.090	-0.149	0.092	-0.070	-0.375	0.024	0.064	-0.074
6.H	0.134	0.090	-0.149	-0.092	0.070	-0.375	-0.024	-0.064	-0.074
7.C	0.000	0.000	0.086	0.000	0.000	-0.040	0.000	0.000	0.176
8.H	0.000	0.000	0.238	0.000	0.000	0.003	0.000	0.000	-0.376
9.H	0.129	0.087	-0.020	-0.089	0.067	0.006	-0.023	-0.061	-0.267
10.H	-0.129	-0.087	-0.020	0.089	-0.067	0.006	0.023	0.061	-0.267

	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.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	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5.H	0.133	-0.282	0.161	0.369	0.056	0.000	0.000	0.379	0.000
6.H	-0.133	0.282	0.161	-0.369	-0.056	0.000	0.000	-0.379	0.000
7.C	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
8.H	0.000	0.000	0.050	0.000	0.000	0.163	0.000	0.000	0.179
9.H	-0.128	0.272	-0.186	0.296	-0.054	-0.081	-0.096	0.270	-0.089
10.H	0.128	-0.272	-0.186	-0.296	0.054	-0.081	0.096	-0.270	-0.089

	10		
1.Re	0.000	0.000	0.000
2.O	0.000	0.000	0.000
3.O	0.000	0.000	0.000
4.C	0.000	0.000	0.000

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     5.H          0.000   0.000   0.000
     6.H          0.000   0.000   0.000
     7.C          0.000   0.000   0.000
     8.H          0.000   0.000   0.407
     9.H         -0.218  -0.280  -0.203
    10.H          0.218   0.280  -0.203

  Largest computed component in inactive x Dipole derivative=  0.7589E-17
  (symmetry index=  2)
  Deviation may result from numerical integration and/or the non-linearity
  in the transformations between Cartesian and Z-matrix coordinates.

  Largest computed component in inactive y Dipole derivative=  0.1735E-17
  (symmetry index=  2)
  Deviation may result from numerical integration and/or the non-linearity
  in the transformations between Cartesian and Z-matrix coordinates.


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

              1           2           3           4           5
6           7           8

           123.7625    186.3363    233.3123    395.3516    495.4477
557.3518    956.0002   1014.8281
         ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1   -0.01485589  0.47492797  0.42615221 -0.11588552 -0.20448564
0.14260930  0.71856749 -0.02625298
    2    0.13237617  0.45913988  0.33194277 -0.12926270 -0.34255854
0.27787334 -0.67096747  0.00237016
    3   -0.55960605  0.45073743 -0.10868577 -0.38132860  0.53361758
-0.16165361 -0.12156950  0.02787026
    4   -0.39628071 -0.47530103  0.74752383 -0.06825670  0.00234917
-0.20516713 -0.10660662  0.01101847
    5    0.02821497  0.07764865  0.16701551  0.41669600  0.36415617
0.23703472 -0.02359986 -0.01412176
    6    0.13254123  0.09766756  0.01019999 -0.05196719 -0.08840364
-0.44493335 -0.03072516 -0.50568155
    7   -0.35719894  0.04280640  0.00403726  0.52771032  0.11018347
0.43445703 -0.01936117 -0.26985745
    8   -0.45111778  0.21491593 -0.17971212  0.45101997 -0.51101942
-0.41626022 -0.02833425  0.16342431
    9   -0.40317623 -0.26621802 -0.27799463 -0.40193787 -0.37733157
0.46405058  0.06422868 -0.14552539
   10    0.00677148 -0.00985647  0.00344130 -0.00195775 -0.00086292
0.05199990  0.02270022  0.78853381

              9          10

           2277.7967   2328.1213
         ----------  ----------
    1    0.00020908 -0.00269763
    2   -0.00141275  0.00271248
    3    0.00407547 -0.00078336
    4    0.00053003 -0.00373547
    5   -0.00731820  0.77591221
    6   -0.69145505  0.17187320
    7   -0.31390244 -0.46846142
    8    0.16253579  0.16200861
```

```
    9   -0.14851170  0.35023007
   10   -0.61221653 -0.00516209


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

                Frequency       Dipole Strength        Absorption
Intensity (degeneracy not counted)
                  cm-1           1e-40 esu2 cm2          km/mole
               ----------          ----------         ----------
               123.762522            0.000017           0.000001
               186.336285            6.985001           0.326244
               233.312278           17.977694           1.051356
               395.351554           15.067152           1.493113
               495.447672            3.474019           0.431428
               557.351795            0.331441           0.046304
               956.000229          673.020616         161.274028
              1014.828111           12.214338           3.106995
              2277.796698            0.219555           0.125353
              2328.121270            0.864679           0.504590



  Zero-Point Energy :      0.050564 a.u.
  ==================       1.375923 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)


                        123.763                       182.658
186.336
               ------------------------      ------------------------
------------------------
     1.Re          0.000   0.000  -0.001          0.029   0.019   0.000
0.000   0.000   0.038
     2.O          -0.033  -0.017   0.020          0.059  -0.061   0.003
0.203  -0.153  -0.032
     3.O           0.033   0.017   0.020          0.059  -0.061  -0.003
-0.203   0.153  -0.032
     4.C           0.000   0.000  -0.039         -0.225   0.142   0.000
0.000   0.000  -0.018
     5.H          -0.015  -0.020  -0.054         -0.378   0.193   0.001
0.192  -0.145  -0.068
     6.H           0.015   0.020  -0.054         -0.378   0.193  -0.001
-0.192   0.145  -0.068
     7.C           0.000   0.000   0.000         -0.146  -0.194   0.000
0.000   0.000  -0.272
     8.H           0.000   0.000  -0.535         -0.439  -0.099   0.000
0.000   0.000  -0.495
     9.H          -0.355  -0.352   0.318         -0.111  -0.365   0.010
0.185  -0.227  -0.355
```

```
    10.H          0.355   0.352   0.318        -0.111  -0.365  -0.010
-0.185   0.227  -0.355


                      210.514                     233.312
281.650
               ------------------------     ------------------------
------------------------
     1.Re        -0.049   0.071   0.000         0.000   0.000  -0.032
-0.070  -0.043   0.000
     2.O          0.205  -0.405  -0.040        -0.079  -0.209   0.041
0.487   0.272  -0.382
     3.O          0.205  -0.405   0.040         0.079   0.209   0.041
0.487   0.272   0.382
     4.C          0.239  -0.046   0.000         0.000   0.000   0.222
-0.125  -0.064   0.000
     5.H          0.454  -0.097   0.008         0.195   0.377   0.493
-0.046  -0.133  -0.019
     6.H          0.454  -0.097  -0.008        -0.195  -0.377   0.493
-0.046  -0.133   0.019
     7.C         -0.102   0.032   0.000         0.000   0.000   0.000
-0.040   0.038   0.000
     8.H         -0.213   0.072   0.000         0.000   0.000  -0.014
-0.049   0.038   0.000
     9.H         -0.113   0.002   0.009        -0.003  -0.003   0.001
-0.064   0.040   0.011
    10.H         -0.113   0.002  -0.009         0.003   0.003   0.001
-0.064   0.040  -0.011


                      395.352                     490.863
495.448
               ------------------------     ------------------------
------------------------
     1.Re         0.000   0.000   0.006        -0.036   0.028   0.000
0.000   0.000   0.013
     2.O          0.064  -0.015  -0.003         0.012  -0.010  -0.011
0.011   0.066   0.012
     3.O         -0.064   0.015  -0.003         0.012  -0.010   0.011
-0.011  -0.066   0.012
     4.C          0.000   0.000  -0.095        -0.020   0.018   0.000
0.000   0.000  -0.269
     5.H         -0.544   0.434   0.064         0.033   0.002   0.000
0.507   0.438   0.097
     6.H          0.544  -0.434   0.064         0.033   0.002   0.000
-0.507  -0.438   0.097
     7.C          0.000   0.000  -0.006         0.339  -0.265   0.000
0.000   0.000   0.007
     8.H          0.000   0.000  -0.035         0.420  -0.294   0.000
0.000   0.000  -0.002
     9.H          0.028  -0.039  -0.016         0.401  -0.335  -0.018
0.015  -0.015   0.000
    10.H         -0.028   0.039  -0.016         0.401  -0.335   0.018
-0.015   0.015   0.000


                      557.352                     572.630
647.173
               ------------------------     ------------------------
------------------------
     1.Re         0.000   0.000  -0.008         0.001  -0.005   0.000
```

```
0.010  -0.003   0.000
     2.O          -0.037   0.012  -0.013         -0.021   0.009   0.000
-0.005   0.002   0.009
     3.O           0.037  -0.012  -0.013         -0.021   0.009   0.000
-0.005   0.002  -0.009
     4.C           0.000   0.000   0.004         -0.110  -0.007   0.000
-0.270   0.158   0.000
     5.H          -0.004  -0.022  -0.012          0.235  -0.171  -0.026
0.577  -0.145  -0.018
     6.H           0.004   0.022  -0.012          0.235  -0.171   0.026
0.577  -0.145   0.018
     7.C           0.000   0.000   0.215          0.105   0.158   0.000
-0.072  -0.079   0.000
     8.H           0.000   0.000  -0.181         -0.578   0.380   0.000
0.272  -0.197   0.000
     9.H           0.524  -0.424  -0.059          0.206  -0.328   0.032
-0.120   0.143  -0.014
    10.H          -0.524   0.424  -0.059          0.206  -0.328  -0.032
-0.120   0.143   0.014


                       694.038                      933.412
956.000
               ------------------------     ------------------------
------------------------
     1.Re         -0.016  -0.035   0.000          0.001  -0.001   0.000
0.000   0.000   0.110
     2.O           0.003   0.015  -0.012          0.011  -0.001   0.010
-0.287  -0.111  -0.608
     3.O           0.003   0.015   0.012          0.011  -0.001  -0.010
0.287   0.111  -0.608
     4.C           0.152   0.288   0.000          0.006   0.002   0.000
0.000   0.000  -0.057
     5.H           0.225   0.594   0.161         -0.012  -0.006  -0.008
-0.039   0.120  -0.001
     6.H           0.225   0.594  -0.161         -0.012  -0.006   0.008
0.039  -0.120  -0.001
     7.C           0.024   0.035   0.000         -0.247   0.164   0.000
0.000   0.000  -0.046
     8.H          -0.108   0.076   0.000          0.521  -0.113   0.000
0.000   0.000   0.069
     9.H           0.043  -0.068   0.010          0.338  -0.355  -0.271
-0.085   0.028   0.006
    10.H           0.043  -0.068  -0.010          0.338  -0.355   0.271
0.085  -0.028   0.006


                       983.716                     1014.828
1016.600
               ------------------------     ------------------------
------------------------
     1.Re         -0.053  -0.021   0.000          0.000   0.000   0.001
0.003   0.001   0.000
     2.O           0.318   0.125   0.573         -0.002   0.000  -0.005
-0.015  -0.006  -0.024
     3.O           0.318   0.125  -0.573          0.002   0.000  -0.005
-0.015  -0.006   0.024
     4.C          -0.005  -0.015   0.000          0.000   0.000  -0.003
0.011   0.015   0.000
     5.H          -0.003  -0.057  -0.011         -0.004   0.004  -0.001
-0.016  -0.021  -0.027
```

```
     6.H         -0.003  -0.057   0.011         0.004  -0.004  -0.001
-0.016  -0.021   0.027
     7.C          0.039   0.038   0.000         0.000   0.000   0.128
0.054   0.111   0.000
     8.H          0.013   0.047   0.000         0.000   0.000  -0.743
0.385  -0.012   0.000
     9.H         -0.149  -0.072   0.141         0.080   0.457  -0.030
-0.383  -0.342   0.390
    10.H         -0.149  -0.072  -0.141        -0.080  -0.457  -0.030
-0.383  -0.342  -0.390


                     1030.660                    2123.140
2197.482
               ------------------------    ------------------------
------------------------
     1.Re        -0.006  -0.011   0.000         0.000   0.000   0.000
0.000  -0.001   0.000
     2.O         -0.002  -0.001  -0.004        -0.001   0.000  -0.001
-0.001  -0.001  -0.001
     3.O         -0.002  -0.001   0.004        -0.001   0.000   0.001
-0.001  -0.001   0.001
     4.C          0.143   0.310   0.000        -0.001   0.000   0.000
0.045   0.130   0.000
     5.H         -0.161  -0.405  -0.498         0.002   0.002  -0.004
-0.112  -0.346   0.599
     6.H         -0.161  -0.405   0.498         0.002   0.002   0.004
-0.112  -0.346  -0.599
     7.C          0.003  -0.010   0.000         0.060  -0.071   0.000
0.001   0.000   0.000
     8.H         -0.046   0.008   0.000         0.221   0.619   0.000
0.001   0.001   0.000
     9.H          0.030   0.029  -0.026        -0.285  -0.101  -0.434
-0.002  -0.001  -0.004
    10.H          0.030   0.029   0.026        -0.285  -0.101   0.434
-0.002  -0.001   0.004


                     2262.275                    2277.797
2328.121
               ------------------------    ------------------------
------------------------
     1.Re         0.000   0.000   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     2.O          0.001   0.000   0.000         0.000   0.000   0.000
0.000   0.000  -0.001
     3.O          0.001   0.000   0.000         0.000   0.000   0.000
0.000   0.000  -0.001
     4.C         -0.001   0.001   0.000         0.000   0.000  -0.001
0.000   0.000  -0.195
     5.H          0.001  -0.001   0.003         0.000  -0.003   0.005
-0.114  -0.357   0.584
     6.H          0.001  -0.001  -0.003         0.000   0.003   0.005
0.114   0.357   0.584
     7.C         -0.125  -0.139   0.000         0.000   0.000  -0.187
0.000   0.000   0.002
     8.H          0.230   0.691   0.000         0.000   0.000  -0.006
0.000   0.000   0.000
     9.H          0.254   0.075   0.383         0.389   0.121   0.562
-0.003  -0.002  -0.005
    10.H          0.254   0.075  -0.383        -0.389  -0.121   0.562
```

```
0.003   0.002  -0.005
```

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
123.762522	0.000017	0.000001
182.657540	81.541441	3.733310
186.336285	6.985001	0.326244
210.513673	92.160118	4.862968
233.312278	17.977694	1.051356
281.650180	14.604869	1.031064
395.351554	15.067152	1.493113
490.863008	67.538693	8.309809
495.447672	3.474019	0.431428
557.351795	0.331441	0.046304
572.629903	79.108350	11.354667
647.173090	94.465219	15.323941
694.038275	35.893367	6.244184
933.411687	1.154451	0.270101
956.000229	673.020616	161.274028
983.716356	218.216902	53.806699
1014.828111	12.214338	3.106995
1016.600163	5.915107	1.507269
1030.659726	45.444263	11.740117
2123.140397	0.623551	0.331840
2197.481944	12.495525	6.882685
2262.274902	2.059579	1.167890
2277.796698	0.219555	0.125353
2328.121270	0.864679	0.504590

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

Pressure:                  1.000000 atm.
Temperature:             298.150000 K
```

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

578.3654	636.5457	645.5008
-0.6439	0.7651	0.0000
0.7651	0.6439	0.0000
0.0000	0.0000	1.0000

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

      298.15   Entropy (cal/mole-K):
42.484    26.966    17.664    87.115
               Internal Energy (Kcal/mole):
0.889     0.889    34.853    36.630
               Constant Volume Heat Capacity (cal/mole-K):
2.981     2.981    21.342    27.304

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