Supplementary Material (ESI) for Dalton Transactions

ReO2MeCH2

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                                          **************************
                                          *  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               1.00782500
     6. H               1.00782500
     7. C              12.00000000
     8. H               1.00782500
     9. H               1.00782500
    10. H               1.00782500



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

Symmetry Displacements

	1			2			3		
1.Re	0.036	0.000	0.000	0.000	0.036	0.000	0.000	0.000	0.000
2.O	-0.110	-0.002	0.000	0.002	-0.120	0.000	0.000	0.000	0.177
3.O	-0.110	-0.002	0.000	0.002	-0.120	0.000	0.000	0.000	-0.177
4.C	-0.116	0.002	0.000	-0.018	-0.104	0.000	0.000	0.000	0.000
5.H	-0.118	0.003	0.000	-0.024	-0.102	0.000	0.000	0.000	0.000
6.H	-0.118	0.003	0.000	-0.024	-0.102	0.000	0.000	0.000	0.000
7.C	-0.108	0.005	0.000	0.012	-0.095	0.000	0.000	0.000	0.000
8.H	-0.105	0.004	0.000	0.023	-0.099	0.000	0.000	0.000	0.000
9.H	-0.108	0.007	0.000	0.010	-0.089	0.000	0.000	0.000	0.000
10.H	-0.108	0.007	0.000	0.010	-0.089	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	0.120	0.013	0.000	0.000	0.089	0.000	0.000	0.000	0.000
3.O	0.120	0.013	0.000	0.000	0.089	0.000	0.000	0.000	0.000
4.C	-0.112	-0.008	0.000	-0.117	-0.138	0.000	0.139	-0.071	0.000
5.H	-0.105	-0.010	0.000	-0.160	-0.124	0.000	-0.537	-0.046	0.000
6.H	-0.105	-0.010	0.000	-0.160	-0.124	0.000	-0.537	-0.046	0.000
7.C	-0.152	-0.020	0.000	0.111	-0.068	0.000	-0.045	0.055	0.000
8.H	-0.166	-0.015	0.000	0.192	-0.096	0.000	0.101	0.005	0.000
9.H	-0.149	-0.028	0.000	0.097	-0.022	0.000	-0.072	0.140	0.000
10.H	-0.149	-0.028	0.000	0.097	-0.022	0.000	-0.072	0.140	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	0.201	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5.H	-0.256	-0.198	0.000	-0.090	0.073	0.000	0.024	-0.367	0.000
6.H	-0.256	-0.198	0.000	-0.090	0.073	0.000	0.024	-0.367	0.000
7.C	0.031	-0.139	0.000	0.138	-0.004	0.000	0.000	0.157	0.000
8.H	0.116	-0.168	0.000	-0.576	0.034	0.000	-0.025	-0.371	0.000
9.H	0.015	-0.089	0.000	-0.445	-0.068	0.000	-0.012	-0.381	0.000
10.H	0.015	-0.089	0.000	-0.445	-0.068	0.000	-0.012	-0.381	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	0.704	0.208	-0.330	0.000	0.000	0.413	0.000
6.H	0.000	0.000	-0.704	0.208	-0.330	0.000	0.000	0.413	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	0.310	-0.130	0.000	0.419	-0.602	0.000
9.H	0.000	0.000	0.000	-0.363	0.395	0.000	-0.210	-0.111	0.000
10.H	0.000	0.000	0.000	-0.363	0.395	0.000	-0.210	-0.111	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

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     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          0.500   0.641   0.000          0.000   0.000   0.000
     9.H         -0.250  -0.321   0.000          0.000   0.000   0.704
    10.H         -0.250  -0.321   0.000          0.000   0.000  -0.704

  Largest computed component in inactive z Dipole derivative=  0.2711E-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

           205.8390    218.7122    282.0957    538.7463    743.4287
789.3156    810.9563    984.2535
         ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1    0.17550018  0.55909538 -0.49173770  0.44364824  0.11113097
-0.18401644  0.16508549  0.37828438
    2    0.51384948 -0.47892752 -0.30416703 -0.34397362  0.15781113
-0.48640732  0.10187696  0.14508998
    3   -0.02005458  0.07248060 -0.53657015  0.02092274 -0.01631867
-0.02256131  0.03172063 -0.83875931
    4    0.59805935  0.13025328  0.55847577  0.37757957 -0.00036933
-0.18112636  0.14507696 -0.34087286
    5   -0.29984238  0.49411343  0.24666324 -0.46922842  0.20679236
-0.56157898  0.10151788 -0.10531636
    6   -0.15356275 -0.09780251 -0.00878185  0.28291022 -0.42236423
-0.53926677 -0.58444257  0.00950828
    7    0.35134272  0.32702185 -0.04449386 -0.41894898 -0.35417413
0.21882290  0.00859676  0.04264837
    8    0.12713326  0.07779244 -0.00069270 -0.05546036  0.22325845
0.08385155 -0.34015503  0.00082626
    9   -0.09076590 -0.08886336  0.03046942  0.12860148  0.47586973
0.01462339 -0.02905133 -0.04600875
   10    0.00140211 -0.00342244 -0.00566855  0.00036226 -0.03793237
0.03213712 -0.03382471 -0.00513804
   11   -0.28424672 -0.23061926  0.03111061  0.17107458 -0.25226832
-0.18002893  0.68074661  0.01673114
   12    0.06998842  0.08951816 -0.03208742 -0.13126526 -0.51936859
0.01841989  0.06705600  0.02157074
   13    0.00133327  0.00241593  0.00168060 -0.00172037  0.05375267
0.02633629 -0.03741733 -0.01568204
   14    0.00727394 -0.00026398  0.00358697 -0.00285929  0.04333122
0.02111904 -0.03681571 -0.00157107

              9          10          11          12          13          14

           1201.5258   1310.3580   1399.9950   2954.7374   3021.8923   3046.5665
         ----------  ----------  ----------  ----------  ----------  ----------
    1   -0.00129951 -0.03298643 -0.01796951  0.00153166  0.00157391 -0.00060318
    2   -0.01863730 -0.04647530 -0.01721422 -0.00219208  0.00351418 -0.00211558
    3    0.02391320  0.00758131  0.00801601 -0.00096114  0.00235929  0.00057695
    4   -0.00185238 -0.02821093 -0.00541097 -0.00045246  0.00419544  0.00163488
    5    0.00485782 -0.07190081 -0.01197868 -0.00136929  0.00726759 -0.00233375
    6   -0.01924034  0.24007781 -0.02743689 -0.00242375 -0.13078639 -0.00168515
```

7	-0.01577250	0.55439784	-0.01955442	-0.00079265	-0.33001909	-0.00037195
8	0.72101634	-0.02636888	-0.24715652	0.15541811	0.02619116	-0.44231279
9	-0.43065452	0.34133335	-0.37720112	-0.25766838	-0.24233987	-0.40914231
10	0.00654881	-0.53609198	-0.00167431	-0.00021355	-0.84192111	0.00635513
11	0.35410187	0.24501843	-0.16729032	0.09462525	-0.17671242	-0.14983043
12	-0.23383147	-0.40133915	-0.44850984	-0.18109647	0.27275135	-0.41192541
13	-0.20120856	-0.00016160	-0.54225745	0.75430744	0.00186780	0.30207022
14	0.26928089	0.00538580	-0.52100718	-0.54653997	0.00465839	0.59458152

Intensities
==========

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
205.839022	71.643911	3.696452
218.712186	109.237122	5.988545
282.095695	14.831052	1.048688
538.746300	73.638390	9.944127
743.428746	108.637714	20.244080
789.315602	91.564895	18.115810
810.956305	98.712063	20.065305
984.253476	198.233968	48.906108
1201.525793	8.333866	2.509907
1310.358036	29.545330	9.704136
1399.995044	21.050517	7.386987
2954.737443	1.441253	1.067425
3021.892306	9.211235	6.977099
3046.566536	2.126552	1.623921

=== AAA ===

Symmetry Displacements

	1			2			3		
1.Re	0.000	0.000	0.036	0.000	0.000	0.000	0.000	0.000	0.000
2.O	0.015	-0.004	-0.120	0.114	0.030	0.088	0.055	-0.070	0.000
3.O	-0.015	0.004	-0.120	-0.114	-0.030	0.088	-0.055	0.070	0.000
4.C	0.000	0.000	-0.109	0.000	0.000	-0.106	0.000	0.000	0.103
5.H	0.009	-0.002	-0.109	0.070	0.018	-0.081	-0.316	-0.043	0.016
6.H	-0.009	0.002	-0.109	-0.070	-0.018	-0.081	0.316	0.043	0.016
7.C	0.000	0.000	-0.092	0.000	0.000	-0.097	0.000	0.000	-0.066
8.H	0.000	0.000	-0.093	0.000	0.000	-0.144	0.000	0.000	0.102
9.H	-0.009	0.002	-0.087	-0.067	-0.018	-0.047	0.305	0.041	-0.282
10.H	0.009	-0.002	-0.087	0.067	0.018	-0.047			

```
-0.305  -0.041  -0.282


                          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   0.101   0.000      0.000   0.000   0.000
0.000   0.000   0.000
     3.O          0.000  -0.101   0.000      0.000   0.000   0.000
0.000   0.000   0.000
     4.C          0.000   0.000  -0.075      0.000   0.000   0.126
0.000   0.000   0.000
     5.H         -0.241  -0.127  -0.198      0.140  -0.113  -0.573
0.038   0.099  -0.116
     6.H          0.241   0.127  -0.198     -0.140   0.113  -0.573
-0.038  -0.099  -0.116
     7.C          0.000   0.000   0.096      0.000   0.000  -0.038
0.000   0.000   0.139
     8.H          0.000   0.000   0.330      0.000   0.000   0.035
0.000   0.000  -0.587
     9.H          0.233   0.122  -0.088     -0.135   0.109   0.031
-0.036  -0.096  -0.417
    10.H         -0.233  -0.122  -0.088      0.135  -0.109   0.031
0.036   0.096  -0.417


                          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          0.187  -0.398   0.227      0.521   0.079   0.000
0.000   0.534   0.000
     6.H         -0.187   0.398   0.227     -0.521  -0.079   0.000
0.000  -0.534   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   0.071      0.000   0.000   0.229
0.000   0.000   0.252
     9.H         -0.181   0.383  -0.263      0.417  -0.076  -0.114
-0.135   0.381  -0.126
    10.H          0.181  -0.383  -0.263     -0.417   0.076  -0.114
0.135  -0.381  -0.126


                         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
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     4.C          0.000   0.000   0.000
     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   0.573
     9.H         -0.308  -0.394  -0.287
    10.H          0.308   0.394  -0.287

  Largest computed component in inactive x Dipole derivative=  0.6288E-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=  0.3469E-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

           172.1320    204.5599    262.2228    535.6349    634.6296
728.3741    959.4060   1395.0022
         ----------  ----------  ----------  ----------  ----------
----------  ----------  ----------
    1   -0.07415808  0.45478845  0.47511252 -0.06542389  0.11689448
0.04750310 -0.73577914 -0.01901026
    2    0.03663585  0.47833210  0.43853421 -0.18852097  0.24172161
0.25455360  0.64702866 -0.01091360
    3   -0.56216522  0.46642554 -0.26159394 -0.19152404 -0.56579169
-0.17917567  0.09087709  0.02808816
    4   -0.42826488 -0.52246640  0.66154702 -0.06466102 -0.20019165
-0.22330809  0.10633403  0.02275063
    5    0.01636210  0.05640070  0.11170708  0.52700186 -0.28708541
0.27175651  0.03180666 -0.02487826
    6    0.13858031  0.08931115  0.02335371 -0.04319765  0.07483598
-0.49845496  0.05451677 -0.51018874
    7   -0.35381159 -0.00862292 -0.02729816  0.50271285  0.04386804
0.40942607  0.00980700 -0.31890408
    8   -0.45342998  0.10507489 -0.13568829  0.34166300  0.62794388
-0.39140332  0.06191957  0.19569852
    9   -0.37870126 -0.22704383 -0.20902593 -0.51985761  0.28886979
0.45058648 -0.11074242 -0.17490062
   10    0.00704201 -0.00452033  0.00278784 -0.00378289 -0.00269581
0.06936938 -0.01547752  0.75280379

              9          10

           3066.9590   3121.7456
         ----------  ----------
    1   -0.00145106  0.00073275
    2   -0.00182582  0.00289897
    3    0.00422691 -0.00387522
    4    0.00300797 -0.00397202
    5   -0.00316156  0.74056168
    6   -0.64047644  0.20706307
    7   -0.33002060 -0.49093167
```

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    8    0.17121704  0.17105057
    9   -0.15291847  0.37199540
   10   -0.65431999 -0.00087979


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

                Frequency       Dipole Strength        Absorption
Intensity (degeneracy not counted)
                  cm-1           1e-40 esu2 cm2          km/mole
               ----------          ----------         ----------
               172.132019            1.394816           0.060181
               204.559886            8.762388           0.449284
               262.222809           30.070662           1.976476
               535.634914           20.090171           2.697308
               634.629575            0.019426           0.003090
               728.374146            0.548261           0.100097
               959.406010          668.127875         160.671962
              1395.002173           21.763516           7.609954
              3066.958978            0.513706           0.394913
              3121.745608            1.831005           1.432733



  Zero-Point Energy :      0.065131 a.u.
  ==================       1.772298 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)


                       172.132                     204.560
205.839
               ------------------------     ------------------------
------------------------
     1.Re         0.000   0.000   0.003         0.000   0.000  -0.031
-0.012  -0.036   0.000
     2.O          0.028   0.003  -0.012        -0.164   0.138   0.023
-0.104   0.156   0.007
     3.O         -0.028  -0.003  -0.012         0.164  -0.138   0.023
-0.104   0.156  -0.007
     4.C          0.000   0.000   0.020         0.000   0.000   0.011
0.160  -0.125   0.000
     5.H          0.012   0.006   0.026        -0.152   0.100   0.042
0.247  -0.157  -0.002
     6.H         -0.012  -0.006   0.026         0.152  -0.100   0.042
0.247  -0.157   0.002
     7.C          0.000   0.000  -0.019         0.000   0.000   0.301
0.196   0.214   0.000
     8.H          0.000   0.000   0.509         0.000   0.000   0.611
0.514   0.109   0.000
     9.H          0.364   0.344  -0.342        -0.097   0.285   0.309
```

```
0.160   0.390  -0.010
    10.H         -0.364  -0.344  -0.342         0.097  -0.285   0.309
0.160   0.390   0.010


                       218.712                    262.223
282.096
               ------------------------     ------------------------
------------------------
     1.Re          0.046  -0.039   0.000         0.000   0.000   0.030
0.072   0.044   0.000
     2.O          -0.107   0.232   0.029         0.076   0.172  -0.032
-0.489  -0.272   0.384
     3.O          -0.107   0.232  -0.029        -0.076  -0.172  -0.032
-0.489  -0.272  -0.384
     4.C          -0.323   0.125   0.000         0.000   0.000  -0.287
0.122   0.065   0.000
     5.H          -0.535   0.180  -0.005        -0.180  -0.335  -0.526
0.038   0.129   0.016
     6.H          -0.535   0.180   0.005         0.180   0.335  -0.526
0.038   0.129  -0.016
     7.C          -0.013  -0.121   0.000         0.000   0.000  -0.012
0.037  -0.037   0.000
     8.H          -0.099  -0.096   0.000         0.000   0.000  -0.017
0.041  -0.035   0.000
     9.H           0.013  -0.191   0.000         0.000  -0.013  -0.008
0.059  -0.038  -0.010
    10.H           0.013  -0.191   0.000         0.000   0.013  -0.008
0.059  -0.038   0.010


                       535.635                    538.746
634.630
               ------------------------     ------------------------
------------------------
     1.Re          0.000   0.000  -0.002         0.033  -0.025   0.000
0.000   0.000  -0.005
     2.O          -0.035   0.002  -0.009        -0.009   0.007   0.008
0.002  -0.029  -0.008
     3.O           0.035  -0.002  -0.009        -0.009   0.007  -0.008
-0.002   0.029  -0.008
     4.C           0.000   0.000   0.084         0.013  -0.012   0.000
0.000   0.000   0.130
     5.H           0.432  -0.532  -0.160        -0.020  -0.003   0.001
-0.601  -0.310  -0.181
     6.H          -0.432   0.532  -0.160        -0.020  -0.003  -0.001
0.601   0.310  -0.181
     7.C           0.000   0.000   0.005        -0.395   0.312   0.000
0.000   0.000  -0.006
     8.H           0.000   0.000   0.018        -0.408   0.310   0.000
0.000   0.000   0.006
     9.H          -0.007   0.020   0.004        -0.388   0.300  -0.004
-0.017   0.011   0.004
    10.H           0.007  -0.020   0.004        -0.388   0.300   0.004
0.017  -0.011   0.004


                       728.374                    743.429
789.316
               ------------------------     ------------------------
------------------------
```

1.Re	0.000	0.000	0.002	0.005	0.007	0.000	0.010	0.027	0.000
2.O	0.022	-0.003	0.019	-0.014	-0.001	-0.003	0.004	-0.010	0.006
3.O	-0.022	0.003	0.019	-0.014	-0.001	0.003	0.004	-0.010	-0.006
4.C	0.000	0.000	0.001	-0.117	-0.102	0.000	-0.064	-0.332	0.000
5.H	0.023	0.008	0.012	0.246	-0.287	-0.032	-0.520	-0.267	-0.036
6.H	-0.023	-0.008	0.012	0.246	-0.287	0.032	-0.520	-0.267	0.036
7.C	0.000	0.000	-0.130	0.062	0.085	0.000	-0.034	-0.046	0.000
8.H	0.000	0.000	0.289	-0.549	0.278	0.000	0.286	-0.143	0.000
9.H	-0.511	0.408	0.145	0.138	-0.358	0.036	-0.074	0.202	-0.023
10.H	0.511	-0.408	0.145	0.138	-0.358	-0.036	-0.074	0.202	0.023

	810.956			959.406			984.253		
1.Re	-0.007	-0.004	0.000	0.000	0.000	0.098	-0.055	-0.021	0.000
2.O	0.001	0.002	-0.007	-0.251	-0.099	-0.539	0.330	0.129	0.593
3.O	0.001	0.002	0.007	0.251	0.099	-0.539	0.330	0.129	-0.593
4.C	0.152	-0.021	0.000	0.000	0.000	-0.064	-0.021	-0.043	0.000
5.H	-0.502	0.245	0.028	-0.091	0.223	0.054	0.037	-0.057	0.014
6.H	-0.502	0.245	-0.028	0.091	-0.223	0.054	0.037	-0.057	-0.014
7.C	0.055	0.064	0.000	0.000	0.000	-0.059	-0.008	0.043	0.000
8.H	-0.396	0.210	0.000	0.000	0.000	0.122	-0.052	0.052	0.000
9.H	0.101	-0.246	0.030	-0.197	0.131	0.054	0.021	-0.102	0.004
10.H	0.101	-0.246	-0.030	0.197	-0.131	0.054	0.021	-0.102	-0.004

	1201.526			1310.358			1395.002		
1.Re	0.000	0.001	0.000	-0.001	-0.002	0.000	0.000	0.000	0.001
2.O	0.000	-0.003	-0.005	0.000	-0.001	0.001	0.000	0.000	-0.001
3.O	0.000	-0.003	0.005	0.000	-0.001	-0.001	0.000	0.000	-0.001
4.C	0.003	0.001	0.000	0.054	0.120	0.000	0.000	0.000	-0.001
5.H	-0.013	-0.003	-0.005	-0.208	-0.526	-0.414			

```
-0.004   0.003   0.000
     6.H         -0.013  -0.003   0.005        -0.208  -0.526   0.414
0.004  -0.003   0.000
     7.C         -0.111   0.074   0.000         0.002  -0.001   0.000
0.000   0.000   0.069
     8.H          0.544  -0.169   0.000        -0.004   0.003   0.000
0.000   0.000  -0.743
     9.H          0.376  -0.379  -0.208        -0.006   0.004   0.004
0.033   0.463  -0.074
    10.H          0.376  -0.379   0.208        -0.006   0.004  -0.004
-0.033  -0.463  -0.074


                     1399.995                    2954.737
3021.892
               ------------------------     ------------------------
------------------------
     1.Re         0.001   0.001   0.000         0.000   0.000   0.000
0.000   0.000   0.000
     2.O         -0.001  -0.001  -0.001         0.000   0.000   0.000
0.000   0.000   0.000
     3.O         -0.001  -0.001   0.001         0.000   0.000   0.000
0.000   0.000   0.000
     4.C         -0.001  -0.001   0.000         0.000   0.000   0.000
0.020   0.060   0.000
     5.H         -0.003   0.001   0.001         0.001   0.001   0.000
-0.111  -0.340   0.608
     6.H         -0.003   0.001  -0.001         0.001   0.001   0.000
-0.111  -0.340  -0.608
     7.C          0.033   0.056   0.000         0.022  -0.041   0.000
0.001   0.000   0.000
     8.H          0.374  -0.084   0.000         0.251   0.692   0.000
-0.001  -0.004   0.000
     9.H         -0.419  -0.327   0.377        -0.255  -0.098  -0.391
-0.002   0.000  -0.003
    10.H         -0.419  -0.327  -0.377        -0.255  -0.098   0.391
-0.002   0.000   0.003


                     3046.567                    3066.959
3121.746
               ------------------------     ------------------------
------------------------
     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   0.001   0.000         0.000   0.000   0.000
0.000   0.000  -0.098
     5.H          0.000  -0.002   0.005         0.001  -0.001   0.001
-0.117  -0.364   0.590
     6.H          0.000  -0.002  -0.005        -0.001   0.001   0.001
0.117   0.364   0.590
     7.C         -0.065  -0.065   0.000         0.000   0.000  -0.093
0.000   0.000   0.000
     8.H          0.206   0.628   0.000         0.000   0.000  -0.021
0.000   0.000   0.000
     9.H          0.279   0.080   0.439         0.398   0.128   0.567
0.000  -0.001  -0.001
```

```
    10.H          0.279   0.080  -0.439        -0.398  -0.128   0.567
0.000   0.001  -0.001
```

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
172.132019	1.394816	0.060181
204.559886	8.762388	0.449284
205.839022	71.643911	3.696452
218.712186	109.237122	5.988545
262.222809	30.070662	1.976476
282.095695	14.831052	1.048688
535.634914	20.090171	2.697308
538.746300	73.638390	9.944127
634.629575	0.019426	0.003090
728.374146	0.548261	0.100097
743.428746	108.637714	20.244080
789.315602	91.564895	18.115810
810.956305	98.712063	20.065305
959.406010	668.127875	160.671962
984.253476	198.233968	48.906108
1201.525793	8.333866	2.509907
1310.358036	29.545330	9.704136
1395.002173	21.763516	7.609954
1399.995044	21.050517	7.386987
2954.737443	1.441253	1.067425
3021.892306	9.211235	6.977099
3046.566536	2.126552	1.623921
3066.958978	0.513706	0.394913
3121.745608	1.831005	1.432733

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

Pressure:                  1.000000 atm.
Temperature:             298.150000 K


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

        523.7326        535.2715        557.4587
-------------------------------------------------
          0.7600          0.0000          0.6499
         -0.6499          0.0000          0.7600
```

```
            0.0000          1.0000          0.0000


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

      298.15   Entropy (cal/mole-K):
42.425    26.549    14.519    83.494
               Internal Energy (Kcal/mole):
0.889     0.889    43.489    45.266
               Constant Volume Heat Capacity (cal/mole-K):
2.981     2.981    18.304    24.265

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