

ReO3C2D5

\*\*\*\*\*  
\* FREQUENCIES \*  
\*\*\*\*\*

Coordinates (Cartesian)

| Atom      | bohr                |                       |           |           |  |
|-----------|---------------------|-----------------------|-----------|-----------|--|
| angstrom  | Geometric Variables |                       |           |           |  |
|           | X                   | Y                     | Z         | X         |  |
| Y         | Z                   | (0:frozen, *:LT par.) |           |           |  |
| 1 Re      | 3.051612            | 0.000000              | 0.000000  | 1.614843  |  |
| 0.000000  | 0.000000            | 1                     | 2         | 3         |  |
| 2 O       | 3.408859            | 1.763826              | 2.717490  | 1.803890  |  |
| 0.933376  | 1.438034            | 4                     | 5         | 6         |  |
| 3 O       | 3.408859            | 1.763826              | -2.717490 | 1.803890  |  |
| 0.933376  | -1.438034           | 7                     | 8         | 9         |  |
| 4 O       | 4.850053            | -2.717966             | 0.000000  | 2.566537  |  |
| -1.438285 | 0.000000            | 10                    | 11        | 12        |  |
| 5 C       | -0.718758           | -1.222714             | 0.000000  | -0.380350 |  |
| -0.647032 | 0.000000            | 13                    | 14        | 15        |  |
| 6 C       | -2.664334           | 0.923189              | 0.000000  | -1.409904 |  |
| 0.488531  | 0.000000            | 16                    | 17        | 18        |  |
| 7 H       | -2.476233           | 2.124797              | -1.680310 | -1.310366 |  |
| 1.124394  | -0.889181           | 19                    | 20        | 21        |  |
| 8 H       | -2.476233           | 2.124797              | 1.680310  | -1.310366 |  |
| 1.124394  | 0.889181            | 22                    | 23        | 24        |  |
| 9 H       | -4.584422           | 0.124934              | 0.000000  | -2.425971 |  |
| 0.066112  | 0.000000            | 25                    | 26        | 27        |  |
| 10 H      | -0.899702           | -2.442345             | 1.678842  | -0.476102 |  |
| -1.292433 | 0.888405            | 28                    | 29        | 30        |  |
| 11 H      | -0.899702           | -2.442345             | -1.678842 | -0.476102 |  |
| -1.292433 | -0.888405           | 31                    | 32        | 33        |  |

Atomic Masses:

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

11. H 2.00000000

Force Constants Matrix: Computed (free variables)

1) 0.4139 -0.1389 0.0000 -0.0442 -0.0323 -0.0626 -0.0442  
-0.0323 0.0626 -0.1901  
0.2322 0.0000 -0.0945 -0.0215 0.0000 -0.0255 0.0010  
0.0000 -0.0001 -0.0002  
-0.0003 -0.0001 -0.0002 0.0003 -0.0008 0.0040 0.0000  
-0.0072 -0.0059 0.0027  
-0.0072 -0.0059 -0.0027

2) -0.1390 0.7987 0.0000 -0.0249 -0.1948 -0.2053 -0.0249  
-0.1948 0.2053 0.2168  
-0.3562 0.0000 -0.0182 -0.0390 0.0000 0.0073 0.0060  
0.0000 0.0026 -0.0004  
0.0009 0.0026 -0.0004 -0.0009 0.0021 -0.0029 0.0000  
-0.0122 -0.0081 0.0009  
-0.0122 -0.0081 -0.0009

3) -0.0005 0.0002 0.8427 -0.0502 -0.2016 -0.3688 0.0503  
0.2016 -0.3689 0.0001  
-0.0002 -0.0624 0.0000 0.0000 -0.0339 0.0000 0.0000  
-0.0020 -0.0030 0.0015  
-0.0003 0.0030 -0.0015 -0.0003 0.0001 0.0000 -0.0010  
0.0172 0.0059 -0.0026  
-0.0171 -0.0059 -0.0026

4) -0.0442 -0.0253 -0.0514 0.0304 0.0292 0.0507 0.0023  
0.0060 -0.0011 0.0103  
-0.0032 0.0131 -0.0020 -0.0067 -0.0118 0.0019 0.0004  
0.0002 0.0000 0.0001  
0.0001 0.0008 -0.0003 -0.0001 0.0005 -0.0010 -0.0005  
0.0024 0.0010 0.0000  
-0.0024 -0.0001 0.0008

5) -0.0316 -0.1940 -0.2001 0.0290 0.1771 0.2175 0.0059  
0.0299 -0.0070 0.0021  
-0.0106 -0.0095 -0.0033 -0.0045 0.0000 0.0000 -0.0005  
-0.0005 0.0000 -0.0001  
-0.0001 -0.0006 0.0003 0.0004 -0.0002 0.0006 0.0005  
-0.0013 0.0006 -0.0013  
-0.0002 0.0011 0.0002

6) -0.0625 -0.2041 -0.3690 0.0503 0.2176 0.3683 0.0015  
0.0063 -0.0189 0.0198  
-0.0201 0.0133 -0.0038 0.0019 0.0055 -0.0030 -0.0029 -0.0002 0.0005  
0.0000  
0.0003 -0.0006 0.0005 0.0001 -0.0006 0.0014 0.0003  
-0.0030 -0.0008 -0.0006  
0.0015 0.0002 0.0009

7) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

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8) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000  
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9) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000  
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10) -0.1907 0.2168 0.0000 0.0105 0.0025 0.0198 0.0105  
0.0025 -0.0198 0.1779  
-0.2296 0.0000 -0.0093 0.0078 0.0000 -0.0001 -0.0021  
0.0000 0.0001 0.0000  
0.0001 0.0001 0.0000 -0.0001 -0.0004 0.0004 0.0000  
0.0007 0.0009 -0.0007  
0.0007 0.0009 0.0007

11) 0.2325 -0.3563 0.0000 -0.0034 -0.0106 -0.0197 -0.0034  
-0.0106 0.0197 -0.2296  
0.3633 0.0000 -0.0015 0.0133 0.0000 -0.0012 -0.0007  
0.0000 -0.0003 -0.0002  
-0.0003 -0.0003 -0.0002 0.0003 -0.0001 -0.0001 0.0000  
0.0036 0.0010 0.0009  
0.0036 0.0010 -0.0009

12) -0.0005 -0.0003 -0.0640 0.0129 -0.0090 0.0137 -0.0129  
0.0092 0.0136 0.0002  
-0.0001 0.0362 0.0001 0.0000 -0.0027 0.0000 0.0000  
0.0014 0.0003 -0.0002  
0.0000 -0.0002 0.0002 0.0000 0.0001 0.0000 0.0000  
0.0002 -0.0004 0.0010  
0.0000 0.0005 0.0010

13) -0.0939 -0.0171 0.0000 -0.0021 -0.0035 -0.0037 -0.0021  
-0.0035 0.0037 -0.0097  
-0.0018 0.0000 0.3089 -0.0236 0.0000 -0.1046 0.0474  
0.0000 -0.0007 -0.0013  
-0.0009 -0.0007 -0.0013 0.0009 -0.0221 0.0248 0.0000  
-0.0365 -0.0101 0.0181  
-0.0365 -0.0101 -0.0181

14) -0.0204 -0.0407 0.0000 -0.0069 -0.0040 0.0020 -0.0069  
-0.0040 -0.0020 0.0077  
0.0134 0.0000 -0.0237 0.4223 0.0000 0.0683 -0.1215  
0.0000 0.0121 -0.0132  
-0.0012 0.0121 -0.0132 0.0012 -0.0023 0.0052 0.0000  
-0.0200 -0.1222 0.1141  
-0.0200 -0.1222 -0.1141

15) -0.0005 -0.0002 -0.0342 -0.0116 0.0002 0.0056 0.0117  
0.0000 0.0056 0.0002  
-0.0001 -0.0029 0.0001 0.0000 0.4981 -0.0003 -0.0001  
-0.0709 -0.0185 0.0172  
0.0016 0.0185 -0.0172 0.0016 0.0003 0.0001 -0.0002  
0.0323 0.1206 -0.2021  
-0.0321 -0.1205 -0.2022

16) -0.0242 0.0075 0.0000 0.0017 -0.0002 -0.0031 0.0017  
-0.0002 0.0031 -0.0005  
-0.0009 0.0000 -0.1049 0.0687 0.0000 0.4632 0.0514  
0.0000 -0.0455 -0.0153  
0.0214 -0.0455 -0.0153 -0.0214 -0.2493 -0.0918 0.0000  
0.0016 -0.0021 0.0005  
0.0016 -0.0021 -0.0005

17) 0.0010 0.0059 0.0000 0.0005 -0.0005 -0.0029 0.0005  
-0.0005 0.0029 -0.0021  
-0.0004 0.0000 0.0471 -0.1218 0.0000 0.0512 0.4774  
0.0000 -0.0162 -0.1260  
0.1179 -0.0162 -0.1260 -0.1179 -0.0941 -0.0807 0.0000  
0.0142 -0.0138 -0.0007  
0.0142 -0.0138 0.0007

18) 0.0001 0.0000 -0.0022 0.0002 -0.0005 -0.0002 -0.0002  
0.0005 -0.0002 0.0000  
0.0000 0.0015 0.0000 0.0000 -0.0708 0.0000 -0.0001  
0.5399 0.0226 0.1171  
-0.2136 -0.0226 -0.1170 -0.2135 0.0000 0.0000 -0.0427  
-0.0184 0.0176 0.0009  
0.0183 -0.0176 0.0008

19) 0.0007 0.0039 -0.0043 -0.0002 -0.0002 0.0007 0.0011  
-0.0011 0.0011 -0.0001  
-0.0006 0.0005 -0.0008 0.0120 -0.0186 -0.0452 -0.0162  
0.0229 0.0504 0.0128  
-0.0232 -0.0010 0.0019 -0.0031 -0.0026 -0.0156 0.0234  
-0.0028 0.0037 0.0000  
0.0004 -0.0008 0.0005

20) -0.0010 -0.0014 0.0025 0.0002 0.0002 -0.0002 -0.0004  
0.0006 -0.0009 0.0002  
0.0000 -0.0005 -0.0010 -0.0130 0.0169 -0.0154 -0.1263  
0.1173 0.0128 0.1375  
-0.1298 0.0020 0.0115 -0.0148 -0.0007 -0.0071 0.0098  
0.0037 -0.0024 -0.0005  
-0.0005 0.0005 0.0000

21) 0.0003 0.0023 -0.0013 -0.0001 -0.0003 0.0005 0.0003  
-0.0008 0.0002 -0.0001  
-0.0004 0.0002 -0.0012 -0.0015 0.0018 0.0209 0.1181  
-0.2138 -0.0231 -0.1297  
0.2287 0.0031 0.0147 -0.0188 0.0001 -0.0014 0.0006  
0.0002 -0.0009 0.0014  
-0.0005 0.0000 0.0006

22) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000  
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24) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000  
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25) -0.0011 0.0019 0.0000 0.0003 0.0000 -0.0005 0.0003  
0.0000 0.0005 -0.0004  
0.0000 0.0000 -0.0218 -0.0021 0.0000 -0.2495 -0.0943  
0.0000 -0.0021 -0.0010  
-0.0003 -0.0021 -0.0010 0.0003 0.2744 0.0970 0.0000  
0.0010 -0.0002 -0.0001  
0.0010 -0.0002 0.0001

26) 0.0038 -0.0018 0.0000 -0.0010 0.0003 0.0013 -0.0010  
0.0003 -0.0013 0.0003  
-0.0003 0.0000 0.0247 0.0053 0.0000 -0.0915 -0.0805  
0.0000 -0.0154 -0.0075  
-0.0012 -0.0154 -0.0075 0.0012 0.0969 0.0894 0.0000  
-0.0008 0.0011 -0.0001  
-0.0008 0.0011 0.0001

27) 0.0000 0.0000 -0.0011 -0.0006 0.0005 0.0003 0.0006  
-0.0005 0.0003 0.0000  
0.0000 0.0000 0.0000 0.0000 -0.0004 -0.0004 -0.0003  
-0.0424 0.0234 0.0099  
0.0004 -0.0234 -0.0097 0.0006 0.0003 0.0001 0.0419  
-0.0003 -0.0003 0.0002

0.0003 0.0003 0.0002

28) -0.0071 -0.0132 0.0185 0.0025 -0.0011 -0.0032 -0.0026  
0.0003 -0.0019 0.0006  
0.0041 -0.0002 -0.0366 -0.0200 0.0323 0.0019 0.0142  
-0.0184 -0.0027 0.0035  
0.0003 0.0005 -0.0006 0.0003 0.0010 -0.0007 -0.0003  
0.0417 0.0108 -0.0232  
0.0006 0.0027 -0.0041

29) -0.0055 -0.0080 0.0072 0.0011 0.0006 -0.0011 -0.0003  
0.0012 -0.0007 0.0007  
0.0011 -0.0007 -0.0099 -0.1225 0.1205 -0.0024 -0.0138  
0.0174 0.0037 -0.0026  
-0.0008 -0.0007 0.0004 -0.0002 0.0000 0.0013 -0.0002  
0.0107 0.1329 -0.1274  
0.0026 0.0093 -0.0142

30) 0.0029 0.0008 -0.0017 0.0000 -0.0012 -0.0008 -0.0007  
-0.0002 0.0008 -0.0010  
0.0009 0.0007 0.0182 0.1141 -0.2024 0.0007 -0.0006  
0.0010 -0.0001 -0.0005  
0.0012 -0.0004 0.0000 0.0005 -0.0005 -0.0001 0.0001  
-0.0231 -0.1273 0.2196  
0.0040 0.0141 -0.0191

31) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000  
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32) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000  
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33) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000  
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Dipole: -1.396556 -0.317086 0.000000  
Derivatives:

1) 1.308927 -0.169441 0.000000

|     |           |           |           |
|-----|-----------|-----------|-----------|
| 2)  | -0.124589 | 1.639096  | -0.000001 |
| 3)  | 0.000603  | 0.000074  | 1.717031  |
| 4)  | -0.242422 | -0.074543 | -0.074668 |
| 5)  | -0.079221 | -0.441355 | -0.444462 |
| 6)  | -0.108930 | -0.425578 | -0.862227 |
| 7)  | 0.000000  | 0.000000  | 0.000000  |
| 8)  | 0.000000  | 0.000000  | 0.000000  |
| 9)  | 0.000000  | 0.000000  | 0.000000  |
| 10) | -0.544606 | 0.445892  | 0.000000  |
| 11) | 0.437339  | -0.906936 | 0.000000  |
| 12) | 0.000735  | 0.000043  | -0.164638 |
| 13) | -0.055714 | -0.074719 | 0.000000  |
| 14) | -0.124798 | -0.028607 | 0.000000  |
| 15) | 0.000089  | 0.000043  | 0.020807  |
| 16) | -0.078949 | -0.003652 | 0.000000  |
| 17) | -0.208849 | 0.042227  | 0.000000  |
| 18) | -0.001297 | -0.001982 | 0.045575  |
| 19) | 0.060923  | -0.011723 | 0.050910  |
| 20) | 0.041187  | 0.013266  | 0.046636  |
| 21) | 0.011903  | 0.066861  | -0.019363 |
| 22) | 0.000000  | 0.000000  | 0.000000  |
| 23) | 0.000000  | 0.000000  | 0.000000  |
| 24) | 0.000000  | 0.000000  | 0.000000  |
| 25) | -0.143506 | -0.021569 | 0.000000  |
| 26) | 0.030572  | 0.038774  | 0.000000  |
| 27) | 0.000194  | 0.000039  | 0.102573  |
| 28) | -0.054846 | -0.005084 | -0.006643 |
| 29) | 0.030313  | 0.031530  | 0.038875  |

30) -0.052539 0.048734 0.024219  
31) 0.000000 0.000000 0.000000  
32) 0.000000 0.000000 0.000000  
33) 0.000000 0.000000 0.000000

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

==== AA ====

Symmetry Displacements

|                    | 1                   | 2                   |
|--------------------|---------------------|---------------------|
| 3                  |                     |                     |
|                    | -----               | -----               |
|                    | -----               |                     |
| 1.Re               | 0.040 0.000 0.000   | 0.000 0.038 0.000   |
| 0.000 0.000 0.000  |                     |                     |
| 2.O                | -0.091 -0.001 0.000 | 0.018 -0.107 0.000  |
| 0.000 0.000 0.177  |                     |                     |
| 3.O                | -0.091 -0.001 0.000 | 0.018 -0.107 0.000  |
| 0.000 0.000 -0.177 |                     |                     |
| 4.O                | -0.094 -0.002 0.000 | -0.031 -0.123 0.000 |
| 0.000 0.000 0.000  |                     |                     |
| 5.C                | -0.093 0.002 0.000  | -0.014 -0.062 0.000 |
| 0.000 0.000 0.000  |                     |                     |
| 6.C                | -0.092 0.004 0.000  | 0.009 -0.041 0.000  |
| 0.000 0.000 0.000  |                     |                     |
| 7.H                | -0.091 0.003 0.000  | 0.022 -0.043 0.000  |
| 0.000 0.000 0.000  |                     |                     |
| 8.H                | -0.091 0.003 0.000  | 0.022 -0.043 0.000  |
| 0.000 0.000 0.000  |                     |                     |
| 9.H                | -0.092 0.005 0.000  | 0.000 -0.020 0.000  |
| 0.000 0.000 0.000  |                     |                     |
| 10.H               | -0.094 0.002 0.000  | -0.028 -0.060 0.000 |
| 0.000 0.000 0.000  |                     |                     |
| 11.H               | -0.094 0.002 0.000  | -0.028 -0.060 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    | 0.128  | 0.025  | 0.000 | 0.000  | 0.122  | 0.000 |
| 0.000  | 0.000  | 0.000  |       |        |        |       |
| 3.O    | 0.128  | 0.025  | 0.000 | 0.000  | 0.122  | 0.000 |
| 0.000  | 0.000  | 0.000  |       |        |        |       |
| 4.O    | -0.059 | 0.043  | 0.000 | -0.032 | -0.160 | 0.000 |
| 0.195  | -0.061 | 0.000  |       |        |        |       |
| 5.C    | -0.078 | -0.029 | 0.000 | -0.005 | -0.060 | 0.000 |
| -0.106 | 0.013  | 0.000  |       |        |        |       |
| 6.C    | -0.106 | -0.054 | 0.000 | 0.034  | -0.025 | 0.000 |
| -0.078 | 0.039  | 0.000  |       |        |        |       |
| 7.H    | -0.121 | -0.051 | 0.000 | 0.056  | -0.028 | 0.000 |
| -0.061 | 0.037  | 0.000  |       |        |        |       |
| 8.H    | -0.121 | -0.051 | 0.000 | 0.056  | -0.028 | 0.000 |
| -0.061 | 0.037  | 0.000  |       |        |        |       |
| 9.H    | -0.096 | -0.078 | 0.000 | 0.020  | 0.010  | 0.000 |
| -0.088 | 0.065  | 0.000  |       |        |        |       |
| 10.H   | -0.063 | -0.031 | 0.000 | -0.027 | -0.057 | 0.000 |
| -0.122 | 0.016  | 0.000  |       |        |        |       |
| 11.H   | -0.063 | -0.031 | 0.000 | -0.027 | -0.057 | 0.000 |
| -0.122 | 0.016  | 0.000  |       |        |        |       |

|        |        |        |       |        |        |       |
|--------|--------|--------|-------|--------|--------|-------|
| 9      | 7      | 8      |       |        |        |       |
| -----  | -----  | -----  |       |        |        |       |
| 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.O    | 0.000  | 0.089  | 0.000 | 0.000  | 0.000  | 0.000 |
| 0.000  | 0.000  | 0.000  |       |        |        |       |
| 5.C    | -0.092 | -0.139 | 0.000 | 0.208  | -0.053 | 0.000 |
| 0.000  | 0.199  | 0.000  |       |        |        |       |
| 6.C    | 0.090  | 0.026  | 0.000 | -0.092 | 0.037  | 0.000 |
| 0.029  | -0.097 | 0.000  |       |        |        |       |
| 7.H    | 0.192  | 0.010  | 0.000 | -0.037 | 0.028  | 0.000 |
| 0.105  | -0.109 | 0.000  |       |        |        |       |
| 8.H    | 0.192  | 0.010  | 0.000 | -0.037 | 0.028  | 0.000 |
| 0.105  | -0.109 | 0.000  |       |        |        |       |
| 9.H    | 0.022  | 0.189  | 0.000 | -0.129 | 0.126  | 0.000 |
| -0.021 | 0.024  | 0.000  |       |        |        |       |
| 10.H   | -0.196 | -0.124 | 0.000 | -0.248 | -0.044 | 0.000 |
| -0.183 | -0.208 | 0.000  |       |        |        |       |
| 11.H   | -0.196 | -0.124 | 0.000 | -0.248 | -0.044 | 0.000 |
| -0.183 | -0.208 | 0.000  |       |        |        |       |

|       |       |       |
|-------|-------|-------|
| 12    | 10    | 11    |
| ----- | ----- | ----- |



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|      |       |       |        |
|------|-------|-------|--------|
| 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.O  | 0.000 | 0.000 | 0.000  |
| 5.C  | 0.000 | 0.000 | 0.000  |
| 6.C  | 0.000 | 0.000 | 0.000  |
| 7.H  | 0.000 | 0.000 | 0.000  |
| 8.H  | 0.000 | 0.000 | 0.000  |
| 9.H  | 0.000 | 0.000 | 0.000  |
| 10.H | 0.000 | 0.000 | 0.500  |
| 11.H | 0.000 | 0.000 | -0.500 |

Frequencies and Normal Modes

=====

|    | 1           | 2           | 3           | 4           | 5           |
|----|-------------|-------------|-------------|-------------|-------------|
| 6  | 7           | 8           |             |             |             |
|    | 124.9211    | 239.6501    | 263.0243    | 318.6741    | 473.4633    |
|    | 696.9227    | 863.2243    | 955.4067    |             |             |
|    | -----       | -----       | -----       | -----       | -----       |
| 1  | -0.14149539 | 0.15053599  | 0.78064312  | 0.08486717  | -0.49436672 |
|    | 0.01668712  | 0.00499274  | 0.17730379  |             |             |
| 2  | -0.33854767 | 0.43568024  | -0.12900232 | -0.45928428 | -0.25102853 |
|    | 0.03270966  | 0.00464384  | -0.62321698 |             |             |
| 3  | 0.00413590  | 0.18081924  | 0.11620110  | -0.56476983 | -0.02227934 |
|    | 0.00506417  | -0.01437962 | 0.43469397  |             |             |
| 4  | -0.73511585 | -0.40946256 | -0.32876817 | 0.01882966  | -0.30919890 |
|    | 0.02572047  | -0.00735125 | 0.28159691  |             |             |
| 5  | -0.12366464 | 0.37119285  | -0.08967861 | 0.67304493  | -0.20577488 |
|    | 0.05730955  | -0.02074081 | -0.13092858 |             |             |
| 6  | 0.20101891  | -0.65980488 | 0.21331948  | -0.07668598 | -0.29899211 |
|    | -0.03009777 | 0.02989252  | -0.48253168 |             |             |
| 7  | 0.51733545  | 0.08301748  | -0.43756395 | -0.05626491 | -0.66362657 |
|    | 0.15711541  | -0.01622666 | 0.19499681  |             |             |
| 8  | -0.00925723 | -0.06060174 | 0.03268020  | -0.00801068 | -0.05785834 |
|    | 0.09811052  | -0.21962005 | 0.11397457  |             |             |
| 9  | -0.01834667 | -0.00516706 | 0.00090503  | 0.01015829  | 0.00317801  |
|    | 0.12456683  | 0.49797975  | 0.06673693  |             |             |
| 10 | -0.01977759 | -0.03280854 | 0.03982096  | -0.01167916 | 0.05440662  |
|    | 0.48667307  | -0.15953786 | -0.04016898 |             |             |
| 11 | -0.00485921 | -0.01204301 | 0.01886649  | -0.00347951 | 0.04572544  |
|    | 0.15726552  | -0.30982338 | -0.03006616 |             |             |
| 12 | 0.00189513  | 0.00040795  | -0.00305734 | 0.00308549  | -0.00899935 |
|    | -0.05939596 | -0.04371371 | 0.02475668  |             |             |
| 13 | 0.00235295  | 0.00874587  | -0.00451640 | 0.00305187  | -0.00319779 |
|    | -0.00473919 | 0.51248499  | 0.02666199  |             |             |
| 14 | -0.00522521 | -0.01805295 | 0.02086135  | -0.00158786 | 0.03958835  |
|    | 0.14807448  | -0.51046808 | 0.00097661  |             |             |
| 15 | -0.02623367 | -0.04201045 | 0.06214830  | -0.01223294 | 0.11946545  |
|    | 0.81040702  | 0.20636510  | -0.02950579 |             |             |
| 16 | 0.00727345  | 0.00773275  | -0.00400389 | -0.00362746 | 0.00265593  |

-0.01128270 0.11282743 -0.04181611

9 10 11 12 13  
 14 15 16

977.9583 987.6107 1023.1527 1051.1393 1096.4982  
 2130.0719 2145.5696 2243.4085

-----  
 -----  
 1 0.05999541 -0.24523454 0.02624445 0.00440021 0.01076465  
 -0.00176942 0.00218429 0.00142545  
 2 0.11970637 -0.01920437 0.01162295 0.01297404 -0.02166960  
 -0.00134169 0.00164075 -0.00156130  
 3 -0.37665031 0.54955438 -0.01748942 -0.00399925 0.03053045  
 0.00018818 -0.00093931 0.00127506  
 4 -0.06863867 -0.05375310 0.01137134 0.00747250 0.00972871  
 -0.00058396 -0.00209626 0.00069706  
 5 -0.25998504 0.50461862 -0.02076538 0.00365806 0.00261784  
 0.00034504 -0.00270107 -0.00011091  
 6 -0.17029870 0.34501240 0.01519550 0.01235549 0.02022845  
 -0.00066948 -0.00098859 0.00102949  
 7 0.02677706 -0.16057840 0.02964671 0.00529734 0.00708349  
 -0.00128454 0.00296467 -0.00126421  
 8 0.66561122 0.37733267 -0.32604804 -0.06480564 -0.47100663  
 -0.01762576 0.05310888 -0.00305456  
 9 0.38050654 0.22492722 0.38592558 -0.18128164 0.34244166  
 -0.04039251 0.48483260 -0.02069963  
 10 -0.01791230 -0.03378571 -0.39310984 -0.32688892 0.41986472  
 0.31368881 -0.02562482 -0.43787668  
 11 -0.16743748 -0.06381832 0.51791055 -0.30027700 -0.40730455  
 -0.22475389 0.16585267 -0.49124477  
 12 0.14692745 0.06897760 -0.10764801 0.52267714 0.29551366  
 -0.58813625 -0.08807894 -0.49165962  
 13 -0.00620341 0.01352296 0.05435709 0.33605720 -0.35196554  
 0.49452078 -0.17794905 -0.46935802  
 14 0.08230840 0.04793125 0.30595332 0.55319570 0.15143675  
 0.43138601 0.29524522 0.10117042  
 15 -0.09882252 -0.04117750 0.04090100 0.22982243 -0.18054815  
 -0.25630457 -0.14900092 0.30430664  
 16 -0.28954608 -0.16736978 -0.45756337 0.14314769 -0.22335147  
 -0.08303187 0.76493691 -0.04039077

Intensities

=====

| Frequency<br>Intensity (degeneracy not counted)<br>cm-1 | Dipole Strength<br>1e-40 esu2 cm2 | Absorption<br>km/mole |
|---|-----------------------------------|-----------------------|
| -----   | -----                             | -----                 |
| 124.921095  | 6.899405                          | 0.216036              |
| 239.650110  | 66.315651                         | 3.983563              |
| 263.024317  | 85.276691                         | 5.622174              |
| 318.674080  | 10.184144                         | 0.813485              |
| 473.463298  | 102.505892                        | 12.165031             |

|             |            |            |
|-------------|------------|------------|
| 696.922653  | 7.767018   | 1.356804   |
| 863.224336  | 11.608923  | 2.511850   |
| 955.406703  | 550.273635 | 131.778652 |
| 977.958304  | 68.579703  | 16.811018  |
| 987.610724  | 47.645929  | 11.794775  |
| 1023.152709 | 13.042428  | 3.344853   |
| 1051.139280 | 16.204224  | 4.269397   |
| 1096.498187 | 0.487827   | 0.134076   |
| 2130.071941 | 13.797984  | 7.366954   |
| 2145.569612 | 6.039770   | 3.248187   |
| 2243.408493 | 2.724598   | 1.532106   |

=== AAA ===

### Symmetry Displacements

|        | 1      | 2      |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|
| 3      |        |        |        |        |        |        |
|        | -----  | -----  |        |        |        |        |
| -----  |        |        |        |        |        |        |
| 1.Re   | 0.000  | 0.000  | 0.038  | 0.000  | 0.000  | 0.000  |
| 0.000  | 0.000  | 0.000  |        |        |        |        |
| 2.O    | 0.030  | 0.000  | -0.107 | 0.060  | 0.092  | 0.097  |
| 0.142  | -0.045 | 0.000  |        |        |        |        |
| 3.O    | -0.030 | 0.000  | -0.107 | -0.060 | -0.092 | 0.097  |
| -0.142 | 0.045  | 0.000  |        |        |        |        |
| 4.O    | 0.000  | 0.000  | -0.124 | 0.000  | 0.000  | -0.104 |
| 0.000  | 0.000  | 0.103  |        |        |        |        |
| 5.C    | 0.000  | 0.000  | -0.062 | 0.000  | 0.000  | -0.031 |
| 0.000  | 0.000  | -0.033 |        |        |        |        |
| 6.C    | 0.000  | 0.000  | -0.040 | 0.000  | 0.000  | -0.061 |
| 0.000  | 0.000  | -0.054 |        |        |        |        |
| 7.H    | -0.019 | 0.000  | -0.042 | -0.037 | -0.057 | -0.106 |
| 0.049  | 0.028  | -0.029 |        |        |        |        |
| 8.H    | 0.019  | 0.000  | -0.042 | 0.037  | 0.057  | -0.106 |
| -0.049 | -0.028 | -0.029 |        |        |        |        |
| 9.H    | 0.000  | 0.000  | -0.018 | 0.000  | 0.000  | 0.008  |
| 0.000  | 0.000  | -0.123 |        |        |        |        |
| 10.H   | 0.019  | 0.000  | -0.060 | 0.037  | 0.057  | 0.014  |
| -0.049 | -0.028 | -0.059 |        |        |        |        |
| 11.H   | -0.019 | 0.000  | -0.060 | -0.037 | -0.057 | 0.014  |
| 0.049  | 0.028  | -0.059 |        |        |        |        |
|        |        |        |        |        |        |        |
|        | 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  | 0.084  | 0.000  | 0.000  | 0.000  | 0.000  |
| 0.000  | 0.000  | 0.000  |        |        |        |        |
| 3.O    | 0.000  | -0.084 | 0.000  | 0.000  | 0.000  | 0.000  |



|      |        |        |        |        |        |        |
|------|--------|--------|--------|--------|--------|--------|
| 6.C  | 0.000  | 0.000  | 0.000  | 0.000  | 0.000  | 0.000  |
| 7.H  | 0.000  | 0.376  | 0.000  | 0.000  | 0.000  | 0.000  |
| 8.H  | 0.000  | -0.376 | 0.000  | 0.000  | 0.000  | 0.000  |
| 9.H  | 0.000  | 0.000  | -0.113 | 0.000  | 0.000  | 0.314  |
| 10.H | 0.124  | 0.289  | 0.057  | -0.344 | 0.240  | -0.157 |
| 11.H | -0.124 | -0.289 | 0.057  | 0.344  | -0.240 | -0.157 |

Frequencies and Normal Modes

|    | 1           | 2           | 3           | 4           | 5           |
|----|-------------|-------------|-------------|-------------|-------------|
| 6  | 7           | 8           |             |             |             |
|    | 72.6236     | 135.6858    | 200.1654    | 320.3901    | 502.0136    |
|    | 668.1328    | 938.4635    | 957.5835    |             |             |
|    |             |             |             |             |             |
| 1  | 0.19583469  | -0.24580978 | -0.43137270 | 0.50029785  | -0.13690542 |
|    | -0.05793608 | 0.15275489  | 0.64703070  |             |             |
| 2  | 0.44339329  | -0.09006976 | -0.30368610 | 0.38499370  | -0.20188690 |
|    | -0.13598125 | -0.18616464 | -0.67849512 |             |             |
| 3  | 0.26462491  | -0.48037591 | -0.40011606 | -0.73111889 | -0.06153799 |
|    | -0.01471330 | 0.01489596  | 0.01792616  |             |             |
| 4  | -0.77548416 | -0.45631965 | -0.30349896 | 0.16999202  | 0.08796876  |
|    | 0.05254404  | -0.04225602 | -0.23853208 |             |             |
| 5  | -0.29686345 | 0.56785508  | -0.43306432 | -0.19432135 | -0.50310157 |
|    | -0.32912555 | -0.03317888 | 0.03885134  |             |             |
| 6  | 0.01869628  | 0.09598697  | -0.15050317 | -0.01132655 | 0.29759892  |
|    | -0.00708513 | -0.61692564 | 0.14293945  |             |             |
| 7  | 0.01185730  | 0.04864796  | -0.06573920 | 0.00027252  | 0.24686945  |
|    | -0.26421436 | 0.41563512  | -0.11847930 |             |             |
| 8  | -0.02403704 | -0.13355805 | 0.17578275  | 0.00664561  | -0.17597352 |
|    | -0.20442616 | 0.32945030  | -0.08362057 |             |             |
| 9  | -0.00881491 | -0.11842915 | 0.13626242  | 0.00129976  | 0.09862747  |
|    | -0.55316664 | 0.22846991  | -0.00478492 |             |             |
| 10 | -0.06110068 | -0.30484867 | 0.40336487  | 0.01059208  | -0.68976152 |
|    | 0.07886150  | -0.18978364 | 0.06804518  |             |             |
| 11 | 0.02534382  | 0.18341459  | -0.20688179 | -0.00161390 | -0.09943497 |
|    | 0.66557463  | 0.43450748  | -0.12709387 |             |             |
|    |             |             |             |             |             |
|    | 9           | 10          | 11          |             |             |
|    | 1044.0249   | 2225.0079   | 2263.1229   |             |             |
|    |             |             |             |             |             |
| 1  | 0.02754329  | -0.00186274 | -0.00119060 |             |             |
| 2  | -0.02403365 | -0.00216282 | 0.00016127  |             |             |
| 3  | 0.00473103  | 0.00398847  | 0.00014677  |             |             |
| 4  | -0.01383280 | 0.00356817  | 0.00109821  |             |             |
| 5  | 0.00353820  | -0.00698092 | -0.00093860 |             |             |
| 6  | 0.04982846  | -0.68245284 | -0.09893661 |             |             |
| 7  | 0.42566684  | -0.13743396 | -0.68959920 |             |             |
| 8  | 0.43471227  | -0.49908332 | 0.56946920  |             |             |
| 9  | -0.73050581 | -0.25386549 | -0.03604403 |             |             |
| 10 | -0.00094990 | -0.18757769 | -0.42742745 |             |             |

11 -0.30355884 -0.40812653 -0.07982709

=====  
 Intensities

| Frequency<br>Intensity (degeneracy not counted)<br>cm-1 | Dipole Strength<br>1e-40 esu2 cm2 | Absorption<br>km/mole |
|---|-----------------------------------|-----------------------|
| 72.623639   | 9.020418                          | 0.164204              |
| 135.685829  | 1.480204                          | 0.050342              |
| 200.165358  | 1.726188                          | 0.086607              |
| 320.390066  | 9.825178                          | 0.789037              |
| 502.013625  | 2.736624                          | 0.344357              |
| 668.132762  | 8.343461                          | 1.397292              |
| 938.463501  | 43.261068                         | 10.176365             |
| 957.583525  | 509.707594                        | 122.342074            |
| 1044.024942   | 19.071588                         | 4.990865              |
| 2225.007860   | 0.019259                          | 0.010741              |
| 2263.122910   | 4.312707                          | 2.446449              |

Zero-Point Energy : 0.056767 a.u.  
 ===== 1.544714 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)

|         | 72.624 | 124.921 |        |        |        |        |
|---------|--------|---------|--------|--------|--------|--------|
| 135.686 |        |         |        |        |        |        |
| 1.Re    | 0.000  | 0.000   | 0.014  | 0.014  | 0.031  | 0.000  |
| 0.000   | 0.000  | -0.015  |        |        |        |        |
| 2.O     | 0.134  | -0.070  | 0.042  | 0.213  | -0.008 | -0.002 |
| -0.132  | -0.041 | 0.029   |        |        |        |        |
| 3.O     | -0.134 | 0.070   | 0.042  | 0.213  | -0.008 | 0.002  |
| 0.132   | 0.041  | 0.029   |        |        |        |        |
| 4.O     | 0.000  | 0.000   | -0.142 | -0.270 | -0.156 | 0.000  |
| 0.000   | 0.000  | 0.038   |        |        |        |        |
| 5.C     | 0.000  | 0.000   | 0.131  | -0.013 | 0.057  | 0.000  |
| 0.000   | 0.000  | -0.004  |        |        |        |        |
| 6.C     | 0.000  | 0.000   | -0.221 | -0.272 | -0.191 | 0.000  |
| 0.000   | 0.000  | 0.059   |        |        |        |        |



|        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|
| 7.H    | -0.007 | -0.303 | -0.438 | -0.441 | -0.169 | -0.002 |
| -0.367 | -0.303 | -0.197 |        |        |        |        |
| 8.H    | 0.007  | 0.303  | -0.438 | -0.441 | -0.169 | 0.002  |
| 0.367  | 0.303  | -0.197 |        |        |        |        |
| 9.H    | 0.000  | 0.000  | -0.059 | -0.165 | -0.451 | 0.000  |
| 0.000  | 0.000  | 0.635  |        |        |        |        |
| 10.H   | -0.034 | 0.236  | 0.300  | 0.097  | 0.023  | -0.009 |
| 0.085  | 0.044  | 0.040  |        |        |        |        |
| 11.H   | 0.034  | -0.236 | 0.300  | 0.097  | 0.023  | 0.009  |
| -0.085 | -0.044 | 0.040  |        |        |        |        |

|         |         |        |         |        |        |        |
|---------|---------|--------|---------|--------|--------|--------|
|         | 200.165 |        | 239.650 |        |        |        |
| 263.024 |         |        |         |        |        |        |
| -----   | -----   |        | -----   |        |        |        |
| -----   |         |        |         |        |        |        |
| 1.Re    | 0.000   | 0.000  | -0.031  | 0.017  | 0.047  | 0.000  |
| 0.092   | -0.015  | 0.000  |         |        |        |        |
| 2.O     | -0.165  | -0.067 | 0.032   | -0.166 | -0.033 | 0.091  |
| -0.337  | -0.016  | 0.060  |         |        |        |        |
| 3.O     | 0.165   | 0.067  | 0.032   | -0.166 | -0.033 | -0.091 |
| -0.337  | -0.016  | -0.060 |         |        |        |        |
| 4.O     | 0.000   | 0.000  | 0.018   | -0.410 | -0.238 | 0.000  |
| -0.016  | -0.109  | 0.000  |         |        |        |        |
| 5.C     | 0.000   | 0.000  | 0.206   | 0.171  | -0.159 | 0.000  |
| -0.058  | 0.253   | 0.000  |         |        |        |        |
| 6.C     | 0.000   | 0.000  | 0.029   | 0.297  | -0.092 | 0.000  |
| -0.270  | 0.086   | 0.000  |         |        |        |        |
| 7.H     | 0.256   | 0.126  | 0.147   | 0.392  | -0.105 | 0.001  |
| -0.441  | 0.104   | -0.004 |         |        |        |        |
| 8.H     | -0.256  | -0.126 | 0.147   | 0.392  | -0.105 | -0.001 |
| -0.441  | 0.104   | 0.004  |         |        |        |        |
| 9.H     | 0.000   | 0.000  | -0.345  | 0.244  | 0.043  | 0.000  |
| -0.157  | -0.196  | 0.000  |         |        |        |        |
| 10.H    | 0.127   | 0.284  | 0.431   | 0.238  | -0.148 | 0.011  |
| -0.042  | 0.244   | -0.006 |         |        |        |        |
| 11.H    | -0.127  | -0.284 | 0.431   | 0.238  | -0.148 | -0.011 |
| -0.042  | 0.244   | 0.006  |         |        |        |        |

|         |         |        |         |        |        |        |
|---------|---------|--------|---------|--------|--------|--------|
|         | 318.674 |        | 320.390 |        |        |        |
| 473.463 |         |        |         |        |        |        |
| -----   | -----   |        | -----   |        |        |        |
| -----   |         |        |         |        |        |        |
| 1.Re    | -0.014  | 0.071  | 0.000   | 0.000  | 0.000  | 0.078  |
| -0.041  | -0.019  | 0.000  |         |        |        |        |
| 2.O     | 0.055   | -0.537 | 0.407   | -0.269 | 0.341  | -0.067 |
| 0.002   | -0.011  | -0.008 |         |        |        |        |
| 3.O     | 0.055   | -0.537 | -0.407  | 0.269  | -0.341 | -0.067 |
| 0.002   | -0.011  | 0.008  |         |        |        |        |
| 4.O     | 0.128   | 0.209  | 0.000   | 0.000  | 0.000  | -0.776 |
| 0.043   | 0.021   | 0.000  |         |        |        |        |
| 5.C     | -0.023  | 0.012  | 0.000   | 0.000  | 0.000  | -0.012 |
| 0.320   | 0.262   | 0.000  |         |        |        |        |
| 6.C     | -0.036  | 0.020  | 0.000   | 0.000  | 0.000  | 0.003  |

|        |        |        |        |        |        |        |  |
|--------|--------|--------|--------|--------|--------|--------|--|
| 0.099  | 0.015  | 0.000  |        |        |        |        |  |
| 7.H    | -0.070 | 0.018  | -0.006 | -0.013 | -0.008 | -0.005 |  |
| -0.123 | 0.032  | -0.009 |        |        |        |        |  |
| 8.H    | -0.070 | 0.018  | 0.006  | 0.013  | 0.008  | -0.005 |  |
| -0.123 | 0.032  | 0.009  |        |        |        |        |  |
| 9.H    | -0.022 | -0.016 | 0.000  | 0.000  | 0.000  | 0.011  |  |
| 0.275  | -0.399 | 0.000  |        |        |        |        |  |
| 10.H   | -0.042 | 0.032  | 0.007  | 0.024  | 0.035  | 0.024  |  |
| 0.463  | 0.242  | 0.003  |        |        |        |        |  |
| 11.H   | -0.042 | 0.032  | -0.007 | -0.024 | -0.035 | 0.024  |  |
| 0.463  | 0.242  | -0.003 |        |        |        |        |  |

|         |         |        |         |        |        |        |  |
|---------|---------|--------|---------|--------|--------|--------|--|
|         | 502.014 |        | 668.133 |        |        |        |  |
| 696.923 |         |        |         |        |        |        |  |
|         | -----   |        | -----   |        |        |        |  |
|         | -----   |        |         |        |        |        |  |
| 1.Re    | 0.000   | 0.000  | -0.008  | 0.000  | 0.000  | 0.003  |  |
| -0.001  | -0.002  | 0.000  |         |        |        |        |  |
| 2.O     | -0.040  | -0.013 | -0.008  | 0.017  | 0.011  | 0.010  |  |
| -0.004  | -0.006  | -0.001 |         |        |        |        |  |
| 3.O     | 0.040   | 0.013  | -0.008  | -0.017 | -0.011 | 0.010  |  |
| -0.004  | -0.006  | 0.001  |         |        |        |        |  |
| 4.O     | 0.000   | 0.000  | -0.004  | 0.000  | 0.000  | 0.003  |  |
| 0.018   | -0.006  | 0.000  |         |        |        |        |  |
| 5.C     | 0.000   | 0.000  | 0.226   | 0.000  | 0.000  | -0.078 |  |
| -0.007  | 0.013   | 0.000  |         |        |        |        |  |
| 6.C     | 0.000   | 0.000  | 0.050   | 0.000  | 0.000  | 0.070  |  |
| -0.149  | -0.026  | 0.000  |         |        |        |        |  |
| 7.H     | 0.224   | -0.284 | -0.130  | 0.203  | -0.242 | -0.084 |  |
| 0.172   | -0.009  | 0.044  |         |        |        |        |  |
| 8.H     | -0.224  | 0.284  | -0.130  | -0.203 | 0.242  | -0.084 |  |
| 0.172   | -0.009  | -0.044 |         |        |        |        |  |
| 9.H     | 0.000   | 0.000  | -0.126  | 0.000  | 0.000  | -0.169 |  |
| -0.382  | 0.524   | 0.000  |         |        |        |        |  |
| 10.H    | -0.210  | -0.494 | -0.165  | 0.605  | -0.068 | -0.054 |  |
| 0.493   | -0.057  | 0.008  |         |        |        |        |  |
| 11.H    | 0.210   | 0.494  | -0.165  | -0.605 | 0.068  | -0.054 |  |
| 0.493   | -0.057  | -0.008 |         |        |        |        |  |

|         |         |        |         |        |        |        |  |
|---------|---------|--------|---------|--------|--------|--------|--|
|         | 863.224 |        | 938.464 |        |        |        |  |
| 955.407 |         |        |         |        |        |        |  |
|         | -----   |        | -----   |        |        |        |  |
|         | -----   |        |         |        |        |        |  |
| 1.Re    | 0.000   | 0.000  | 0.000   | 0.000  | 0.000  | 0.010  |  |
| 0.029   | -0.096  | 0.000  |         |        |        |        |  |
| 2.O     | 0.002   | 0.005  | 0.004   | -0.008 | -0.036 | -0.059 |  |
| 0.035   | 0.234   | 0.313  |         |        |        |        |  |
| 3.O     | 0.002   | 0.005  | -0.004  | 0.008  | 0.036  | -0.059 |  |
| 0.035   | 0.234   | -0.313 |         |        |        |        |  |
| 4.O     | -0.011  | 0.001  | 0.000   | 0.000  | 0.000  | -0.002 |  |
| -0.424  | 0.635   | 0.000  |         |        |        |        |  |
| 5.C     | 0.079   | -0.191 | 0.000   | 0.000  | 0.000  | -0.181 |  |
| 0.114   | 0.052   | 0.000  |         |        |        |        |  |

|        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|
| 6.C    | -0.002 | 0.190  | 0.000  | 0.000  | 0.000  | 0.204  |
| -0.070 | -0.030 | 0.000  |        |        |        |        |
| 7.H    | -0.414 | 0.331  | 0.037  | 0.290  | -0.370 | -0.008 |
| 0.077  | 0.015  | 0.050  |        |        |        |        |
| 8.H    | -0.414 | 0.331  | -0.037 | -0.290 | 0.370  | -0.008 |
| 0.077  | 0.015  | -0.050 |        |        |        |        |
| 9.H    | 0.076  | 0.003  | 0.000  | 0.000  | 0.000  | -0.094 |
| -0.126 | 0.096  | 0.000  |        |        |        |        |
| 10.H   | 0.184  | -0.364 | -0.094 | -0.350 | 0.332  | 0.003  |
| -0.094 | -0.040 | -0.085 |        |        |        |        |
| 11.H   | 0.184  | -0.364 | 0.094  | 0.350  | -0.332 | 0.003  |
| -0.094 | -0.040 | 0.085  |        |        |        |        |

|         |         |        |         |        |        |        |
|---------|---------|--------|---------|--------|--------|--------|
|         | 957.584 |        | 977.958 |        |        |        |
| 987.611 |         |        |         |        |        |        |
|         | -----   |        | -----   |        |        |        |
|         | -----   |        |         |        |        |        |
| 1.Re    | 0.000   | 0.000  | -0.088  | -0.005 | -0.009 | 0.000  |
| -0.028  | -0.002  | 0.000  |         |        |        |        |
| 2.O     | 0.067   | 0.299  | 0.486   | 0.025  | 0.094  | 0.136  |
| 0.043   | 0.179   | 0.279  |         |        |        |        |
| 3.O     | -0.067  | -0.299 | 0.486   | 0.025  | 0.094  | -0.136 |
| 0.043   | 0.179   | -0.279 |         |        |        |        |
| 4.O     | 0.000   | 0.000  | 0.030   | 0.062  | -0.075 | 0.000  |
| 0.224   | -0.332  | 0.000  |         |        |        |        |
| 5.C     | 0.000   | 0.000  | -0.063  | -0.314 | -0.092 | 0.000  |
| 0.234   | 0.068   | 0.000  |         |        |        |        |
| 6.C     | 0.000   | 0.000  | 0.116   | 0.090  | 0.092  | 0.000  |
| -0.087  | -0.058  | 0.000  |         |        |        |        |
| 7.H     | 0.105   | -0.197 | -0.006  | -0.065 | -0.099 | -0.150 |
| 0.087   | 0.054   | 0.099  |         |        |        |        |
| 8.H     | -0.105  | 0.197  | -0.006  | -0.065 | -0.099 | 0.150  |
| 0.087   | 0.054   | -0.099 |         |        |        |        |
| 9.H     | 0.000   | 0.000  | -0.115  | 0.254  | -0.292 | 0.000  |
| -0.196  | 0.194   | 0.000  |         |        |        |        |
| 10.H    | -0.282  | 0.144  | -0.001  | 0.398  | 0.219  | 0.296  |
| -0.344  | -0.196  | -0.240 |         |        |        |        |
| 11.H    | 0.282   | -0.144 | -0.001  | 0.398  | 0.219  | -0.296 |
| -0.344  | -0.196  | 0.240  |         |        |        |        |

|          |          |        |          |       |        |        |
|----------|----------|--------|----------|-------|--------|--------|
|          | 1023.153 |        | 1044.025 |       |        |        |
| 1051.139 |          |        |          |       |        |        |
|          | -----    |        | -----    |       |        |        |
|          | -----    |        |          |       |        |        |
| 1.Re     | -0.002   | -0.001 | 0.000    | 0.000 | 0.000  | -0.002 |
| 0.000    | -0.001   | 0.000  |          |       |        |        |
| 2.O      | 0.001    | 0.005  | 0.005    | 0.000 | 0.005  | 0.008  |
| -0.001   | 0.001    | 0.001  |          |       |        |        |
| 3.O      | 0.001    | 0.005  | -0.005   | 0.000 | -0.005 | 0.008  |
| -0.001   | 0.001    | -0.001 |          |       |        |        |
| 4.O      | 0.000    | -0.006 | 0.000    | 0.000 | 0.000  | 0.001  |
| -0.002   | 0.003    | 0.000  |          |       |        |        |
| 5.C      | 0.118    | -0.141 | 0.000    | 0.000 | 0.000  | -0.012 |

|        |        |        |        |        |        |        |  |
|--------|--------|--------|--------|--------|--------|--------|--|
| 0.024  | 0.051  | 0.000  |        |        |        |        |  |
| 6.C    | 0.054  | -0.084 | 0.000  | 0.000  | 0.000  | -0.110 |  |
| 0.090  | 0.060  | 0.000  |        |        |        |        |  |
| 7.H    | -0.265 | 0.088  | 0.084  | 0.478  | 0.099  | 0.024  |  |
| -0.265 | -0.427 | -0.383 |        |        |        |        |  |
| 8.H    | -0.265 | 0.088  | -0.084 | -0.478 | -0.099 | 0.024  |  |
| -0.265 | -0.427 | 0.383  |        |        |        |        |  |
| 9.H    | -0.164 | 0.405  | 0.000  | 0.000  | 0.000  | 0.714  |  |
| -0.054 | 0.383  | 0.000  |        |        |        |        |  |
| 10.H   | -0.100 | 0.399  | 0.358  | 0.014  | 0.008  | -0.009 |  |
| -0.024 | -0.085 | -0.105 |        |        |        |        |  |
| 11.H   | -0.100 | 0.399  | -0.358 | -0.014 | -0.008 | -0.009 |  |
| -0.024 | -0.085 | 0.105  |        |        |        |        |  |

|          |          |        |          |        |        |        |  |
|----------|----------|--------|----------|--------|--------|--------|--|
|          | 1096.498 |        | 2130.072 |        |        |        |  |
| 2145.570 |          |        |          |        |        |        |  |
|          | -----    |        | -----    |        |        |        |  |
| 1.Re     | 0.001    | -0.002 | 0.000    | 0.000  | 0.000  | 0.000  |  |
| 0.000    | 0.000    | 0.000  |          |        |        |        |  |
| 2.O      | 0.000    | 0.006  | 0.011    | 0.000  | 0.000  | 0.000  |  |
| 0.001    | 0.001    | 0.000  |          |        |        |        |  |
| 3.O      | 0.000    | 0.006  | -0.011   | 0.000  | 0.000  | 0.000  |  |
| 0.001    | 0.001    | 0.000  |          |        |        |        |  |
| 4.O      | 0.006    | 0.004  | 0.000    | 0.000  | 0.000  | 0.000  |  |
| 0.000    | -0.001   | 0.000  |          |        |        |        |  |
| 5.C      | -0.211   | 0.192  | 0.000    | -0.005 | -0.010 | 0.000  |  |
| -0.016   | -0.138   | 0.000  |          |        |        |        |  |
| 6.C      | 0.265    | -0.270 | 0.000    | 0.086  | -0.061 | 0.000  |  |
| -0.007   | 0.019    | 0.000  |          |        |        |        |  |
| 7.H      | -0.321   | 0.238  | 0.305    | 0.053  | 0.303  | -0.427 |  |
| -0.008   | -0.043   | 0.065  |          |        |        |        |  |
| 8.H      | -0.321   | 0.238  | -0.305   | 0.053  | 0.303  | 0.427  |  |
| -0.008   | -0.043   | -0.065 |          |        |        |        |  |
| 9.H      | 0.021    | 0.323  | 0.000    | -0.597 | -0.259 | 0.000  |  |
| 0.027    | 0.009    | 0.000  |          |        |        |        |  |
| 10.H     | 0.085    | -0.150 | -0.230   | 0.006  | 0.042  | -0.060 |  |
| 0.064    | 0.397    | -0.567 |          |        |        |        |  |
| 11.H     | 0.085    | -0.150 | 0.230    | 0.006  | 0.042  | 0.060  |  |
| 0.064    | 0.397    | 0.567  |          |        |        |        |  |

|          |          |       |          |       |       |       |  |
|----------|----------|-------|----------|-------|-------|-------|--|
|          | 2225.008 |       | 2243.408 |       |       |       |  |
| 2263.123 |          |       |          |       |       |       |  |
|          | -----    |       | -----    |       |       |       |  |
| 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    | 0.000 |          |       |       |       |  |
| 3.O      | 0.001    | 0.000 | 0.000    | 0.000 | 0.000 | 0.000 |  |
| 0.000    | 0.000    | 0.000 |          |       |       |       |  |
| 4.O      | 0.000    | 0.000 | -0.001   | 0.000 | 0.000 | 0.000 |  |
| 0.000    | 0.000    | 0.000 |          |       |       |       |  |

|        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|
| 5.C    | 0.000  | 0.000  | 0.186  | 0.001  | 0.006  | 0.000  |
| 0.000  | 0.000  | 0.027  |        |        |        |        |
| 6.C    | 0.000  | 0.000  | -0.033 | 0.126  | 0.138  | 0.000  |
| 0.000  | 0.000  | 0.187  |        |        |        |        |
| 7.H    | -0.018 | -0.059 | 0.091  | -0.040 | -0.261 | 0.377  |
| 0.068  | 0.395  | -0.556 |        |        |        |        |
| 8.H    | 0.018  | 0.059  | 0.091  | -0.040 | -0.261 | -0.377 |
| -0.068 | -0.395 | -0.556 |        |        |        |        |
| 9.H    | 0.000  | 0.000  | -0.003 | -0.674 | -0.288 | 0.000  |
| 0.000  | 0.000  | 0.007  |        |        |        |        |
| 10.H   | 0.074  | 0.400  | -0.552 | -0.001 | -0.027 | 0.031  |
| 0.004  | 0.071  | -0.089 |        |        |        |        |
| 11.H   | -0.074 | -0.400 | -0.552 | -0.001 | -0.027 | -0.031 |
| -0.004 | -0.071 | -0.089 |        |        |        |        |

List of All Frequencies:

Intensities

| Frequency                          | Dipole Strength                        | Absorption |
|------------------------------------|--|------------|
| Intensity (degeneracy not counted) | 1e-40 esu <sup>2</sup> cm <sup>2</sup> | km/mole    |
| cm <sup>-1</sup>                   |  |            |
| -----                              | -----                                  | -----      |
| 72.623639                          | 9.020418                               | 0.164204   |
| 124.921095                         | 6.899405                               | 0.216036   |
| 135.685829                         | 1.480204                               | 0.050342   |
| 200.165358                         | 1.726188                               | 0.086607   |
| 239.650110                         | 66.315651                              | 3.983563   |
| 263.024317                         | 85.276691                              | 5.622174   |
| 318.674080                         | 10.184144                              | 0.813485   |
| 320.390066                         | 9.825178                               | 0.789037   |
| 473.463298                         | 102.505892                             | 12.165031  |
| 502.013625                         | 2.736624                               | 0.344357   |
| 668.132762                         | 8.343461                               | 1.397292   |
| 696.922653                         | 7.767018                               | 1.356804   |
| 863.224336                         | 11.608923                              | 2.511850   |
| 938.463501                         | 43.261068                              | 10.176365  |
| 955.406703                         | 550.273635                             | 131.778652 |
| 957.583525                         | 509.707594                             | 122.342074 |
| 977.958304                         | 68.579703                              | 16.811018  |
| 987.610724                         | 47.645929                              | 11.794775  |
| 1023.152709                        | 13.042428                              | 3.344853   |
| 1044.024942                        | 19.071588                              | 4.990865   |
| 1051.139280                        | 16.204224                              | 4.269397   |
| 1096.498187                        | 0.487827                               | 0.134076   |
| 2130.071941                        | 13.797984                              | 7.366954   |
| 2145.569612                        | 6.039770                               | 3.248187   |
| 2225.007860                        | 0.019259                               | 0.010741   |
| 2243.408493                        | 2.724598                               | 1.532106   |
| 2263.122910                        | 4.312707                               | 2.446449   |

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

Pressure: 1.000000 atm.  
Temperature: 298.150000 K

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

|          |           |           |
|----------|-----------|-----------|
| 537.3355 | 1127.7716 | 1147.4974 |
| -----    |           |           |
| 0.9923   | 0.1235    | 0.0000    |
| -0.1235  | 0.9923    | 0.0000    |
| 0.0000   | 0.0000    | 1.0000    |

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

|        |   |        |        |
|--------|---|--------|--------|
| 298.15 | Entropy (cal/mole-K):                       |        |        |
| 42.667 | 28.033                                      | 21.219 | 91.919 |
|        | Internal Energy (Kcal/mole):                |        |        |
| 0.889  | 0.889                                       | 39.118 | 40.895 |
|        | Constant Volume Heat Capacity (cal/mole-K): |        |        |
| 2.981  | 2.981                                       | 22.695 | 28.657 |

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