

**A**

tmaG005

|  |   |   |
|--|---|---|
| b3lyp -405.3050421<br>ccsd(t) -404.192567<br>mp2(3df,2p) -404.2586909<br>mp2(d,p) -404.0142883<br>-----<br>ZPE 0.202497<br>Thermal 0.2120089<br>S2: 0.757431<br>-----<br>G2M(MP2,cc) Energy (0K): -404.2344726<br>G2M(MP2,cc) Enthalpy (298K): -404.2249607<br>T1 Diag: 0.03519514 | Geometry:<br><br>C -1.307656 0.647168 0.000000<br>C 0.004480 0.165898 0.000000<br>C 1.095323 1.032700 0.000000<br>C 0.871659 2.417729 0.000000<br>C -0.431840 2.839263 0.000000<br>C -1.538747 2.025409 0.000000<br>H -2.550121 2.414268 0.000000<br>H 1.708550 3.106103 0.000000<br>H 2.116502 0.680775 0.000000<br>H -2.160924 -0.019895 0.000000<br>N 0.203684 -1.335277 0.000000<br>C -0.431840 -1.935719 1.238904<br>C -0.431840 -1.935719 -1.238904<br>C 1.659164 -1.734362 0.000000<br>H 0.032219 -1.486743 2.114625<br>H -1.497372 -1.726238 1.236709<br>H -0.264102 -3.011611 1.226459<br>H 0.032219 -1.486743 -2.114625<br>H -1.497372 -1.726238 -1.236709<br>H -0.264102 -3.011611 -1.226459<br>H 2.141528 -1.348882 -0.894943<br>H 1.703438 -2.821577 0.000000<br>H 2.141528 -1.348882 0.894943 | Frequencies:<br><br>57.1993 141.8994 227.6378<br>255.2958 285.5207 335.1916<br>344.8993 352.3355 374.5015<br>403.8620 423.2738 473.3759<br>530.7031 561.1267 609.8136<br>699.6290 703.5925 804.1257<br>807.4306 836.2507 934.3902<br>955.3847 955.8971 967.9910<br>992.5494 1053.2437 1072.8831<br>1106.0153 1121.5280 1136.2680<br>1144.1609 1196.0781 1252.6249<br>1254.5784 1289.4120 1310.6569<br>1335.9073 1413.2714 1445.4012<br>1446.3708 1477.3500 1480.4837<br>1486.5501 1489.3977 1494.1976<br>1506.9195 1512.4525 1526.9456<br>1573.0659 1636.4140 3076.0356<br>3076.7996 3084.0082 3165.8929<br>3166.3528 3173.4539 3179.8933<br>3180.6973 3186.2283 3188.4456<br>3190.5495 3197.0277 3224.4534 |
|--|---|---|

**B**

tmaG101

|   |  |   |
|---|--|---|
| <p>b3lyp -555.7417728<br/>                     ccscd(t) -554.2980929<br/>                     mp2(3df,2p) -554.4714127<br/>                     mp2(d,p) -554.1326616<br/>                     -----<br/>                     ZPE 0.2108158<br/>                     Thermal 0.222416<br/>                     S2: 0.755845<br/>                     -----<br/>                     G2M(MP2,cc) Energy (OK): -554.4260282<br/>                     G2M(MP2,cc) Enthalpy (298K): -554.4144280<br/>                     T1 Diag: 0.01869046</p> | <p>Geometry:</p> <p>C 2.078788 -0.227119 0.000028<br/>                     C 1.306664 -1.385495 0.000025<br/>                     C -0.075590 -1.272593 0.000047<br/>                     C -0.668853 -0.007679 0.000101<br/>                     C 0.116682 1.142173 0.000050<br/>                     C 1.505550 1.035908 0.000029<br/>                     H 1.788785 -2.355043 -0.000010<br/>                     H -0.662952 -2.181480 -0.000004<br/>                     H -0.310781 2.133656 0.000000<br/>                     H 2.132941 1.916159 -0.000005<br/>                     C -2.687790 1.493376 -0.000225<br/>                     C -2.726343 -0.608624 -1.239293<br/>                     H -2.341015 2.003586 0.895143<br/>                     H -2.438924 -1.655920 -1.233824<br/>                     N -2.177598 0.072452 0.000000<br/>                     H -3.811804 -0.521309 -1.229290<br/>                     H -2.311308 -0.113986 -2.115054<br/>                     H -2.340270 2.003571 -0.895315<br/>                     H -3.774979 1.453000 -0.000672<br/>                     C -2.726574 -0.608297 1.239377<br/>                     H -2.439176 -1.655597 1.234257<br/>                     H -2.311703 -0.113424 2.115084<br/>                     H -3.812031 -0.520977 1.229150<br/>                     O 3.454152 -0.441252 -0.000012<br/>                     O 4.188497 0.657589 -0.000026</p> | <p>Frequencies:</p> <p>48.9567 71.9015 115.3834<br/>                     187.3609 207.8508 262.7309<br/>                     265.9898 272.8110 337.2696<br/>                     355.9014 356.9804 391.7952<br/>                     422.9892 450.5427 474.6805<br/>                     488.4566 551.0348 588.5086<br/>                     641.5408 682.7800 722.7654<br/>                     819.7710 824.0289 847.4222<br/>                     851.6389 936.6939 954.2868<br/>                     969.5636 986.3033 1021.0346<br/>                     1073.8838 1119.5167 1125.5891<br/>                     1135.9286 1143.4658 1155.9296<br/>                     1160.4269 1227.3257 1252.5965<br/>                     1254.2705 1290.7957 1339.1368<br/>                     1354.9806 1443.2819 1446.5045<br/>                     1454.0558 1477.4880 1485.1391<br/>                     1488.1865 1491.1512 1506.5996<br/>                     1512.9109 1523.4725 1528.2189<br/>                     1628.5954 1643.9829 3076.3863<br/>                     3077.3626 3084.1015 3166.6265<br/>                     3167.0406 3174.0970 3180.8544<br/>                     3185.5294 3186.6424 3198.3230<br/>                     3210.4990 3223.2985 3234.2836</p> |
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**H**

tmaG303

|   |   |   |
|---|---|---|
| <p>b3lyp -555.81036<br/>                     ccscd(t) -554.3634943<br/>                     mp2(3df,2p) -554.5180705<br/>                     mp2(d,p) -554.1750922<br/>                     -----<br/>                     ZPE 0.2102886<br/>                     Thermal 0.2221841<br/>                     S2: 0.77734<br/>                     -----<br/>                     G2M(MP2,cc) Energy (OK): -554.4961840<br/>                     G2M(MP2,cc) Enthalpy (298K): -554.4842885<br/>                     T1 Diag: 0.03008259</p> | <p>Geometry:</p> <p>C -1.346847 1.733184 0.000008<br/>                     C -2.687764 -0.379084 -0.000102<br/>                     C -0.027830 1.363527 -0.000021<br/>                     C -1.569255 -1.322796 0.000025<br/>                     C 0.520700 0.066153 0.000022<br/>                     C -0.213376 -1.135115 0.000056<br/>                     H -1.584194 2.790510 0.000012<br/>                     H -1.933347 -2.342541 0.000068<br/>                     H 0.626340 2.221273 -0.000051<br/>                     H 0.347961 -2.061942 0.000081<br/>                     O -2.477872 1.025854 0.000045<br/>                     O -3.827303 -0.720607 0.000003<br/>                     N 2.032614 -0.091758 -0.000004<br/>                     C 2.473293 -0.846607 1.242222<br/>                     C 2.473165 -0.847040 -1.242011<br/>                     C 2.777116 1.223709 -0.000252<br/>                     H 2.144879 -0.287989 2.116389<br/>                     H 2.029158 -1.837334 1.247352<br/>                     H 3.559102 -0.929225 1.227889<br/>                     H 2.144705 -0.288699 -2.116338<br/>                     H 2.028965 -1.837742 -1.246765<br/>                     H 3.558970 -0.929712 -1.227740<br/>                     H 2.527283 1.785926 -0.896680<br/>                     H 3.840881 0.995897 -0.000154<br/>                     H 2.527186 1.786315 0.895907</p> | <p>Frequencies:</p> <p>28.4203 55.5862 80.2218<br/>                     178.4444 223.4787 231.5774<br/>                     266.9946 292.8426 343.6460<br/>                     363.3393 364.5416 386.9694<br/>                     389.6431 452.5646 461.5805<br/>                     478.9105 543.1141 578.3919<br/>                     623.1696 676.7370 687.6448<br/>                     764.1634 803.4511 811.7625<br/>                     822.2431 873.2185 926.1445<br/>                     931.8587 949.0562 971.8209<br/>                     1043.0521 1063.4541 1071.2209<br/>                     1108.4580 1132.8934 1139.7281<br/>                     1245.9343 1247.6121 1272.0888<br/>                     1289.9260 1354.1788 1379.9823<br/>                     1438.0343 1447.2865 1453.9609<br/>                     1468.5064 1476.8391 1486.3953<br/>                     1489.5618 1493.1393 1509.6807<br/>                     1513.6934 1527.5127 1537.2946<br/>                     1600.9988 1836.5619 3075.8295<br/>                     3076.5305 3083.9349 3165.2205<br/>                     3165.3452 3173.3847 3173.6097<br/>                     3181.2829 3187.7101 3194.0484<br/>                     3196.8503 3204.5913 3238.1543</p> |
|---|---|---|

**N**

tmaG901

|   |  |   |
|---|--|---|
| <p>b3lyp -555.7845343<br/>                     ccscd(t) -554.339744<br/>                     mp2(3df,2p) -554.4885064<br/>                     mp2(d,p) -554.1522375<br/>                     -----<br/>                     ZPE 0.2069682<br/>                     Thermal 0.2202138<br/>                     S2: 0.771626<br/>                     -----<br/>                     G2M(MP2,cc) Energy (OK): -554.4690447<br/>                     G2M(MP2,cc) Enthalpy (298K): -554.4557991<br/>                     T1 Diag: 0.03085654</p> | <p>Geometry:</p> <p>C 1.443279 -1.759587 0.526550<br/>                     C 2.459728 -1.295185 -0.216788<br/>                     C 1.604404 1.512138 0.462483<br/>                     C 0.118185 -1.255108 0.603741<br/>                     C -0.380843 -0.029514 0.133594<br/>                     C 0.310515 1.138378 -0.120426<br/>                     H 1.682166 -2.689337 1.035422<br/>                     H -0.122415 1.941644 -0.698877<br/>                     H -0.567728 -1.952291 1.066956<br/>                     O 3.358024 -0.929846 -0.827910<br/>                     O 2.153680 2.552951 0.168953<br/>                     H 2.030256 0.845400 1.233841<br/>                     N -1.906432 -0.028779 -0.104075<br/>                     C -2.300678 -1.165842 -1.023670<br/>                     C -2.615883 -0.171078 1.227926<br/>                     C -2.408323 1.248274 -0.737661<br/>                     H -1.771088 -1.045122 -1.966700<br/>                     H -2.034281 -2.115620 -0.570202<br/>                     H -3.376684 -1.121204 -1.185263<br/>                     H -2.304618 0.649062 1.871655<br/>                     H -2.358820 -1.122214 1.684620<br/>                     H -3.689833 -0.129198 1.051691<br/>                     H -2.190124 2.091025 -0.087287<br/>                     H -3.485086 1.148843 -0.858877<br/>                     H -1.942658 1.380781 -1.711285</p> | <p>Frequencies:</p> <p>44.0890 56.0597 82.0987<br/>                     120.5153 143.4397 206.9023<br/>                     213.3012 230.3438 237.4719<br/>                     271.6789 309.6582 351.6219<br/>                     363.3311 367.7148 384.4797<br/>                     425.7924 447.7158 483.1908<br/>                     536.7277 565.0456 604.1941<br/>                     651.3111 713.8305 803.6005<br/>                     810.7422 827.7023 886.9385<br/>                     937.2564 944.7958 958.2182<br/>                     1014.0606 1052.8406 1072.2222<br/>                     1125.0077 1132.5143 1154.9460<br/>                     1210.5317 1249.5013 1256.6496<br/>                     1275.5796 1337.8949 1407.3697<br/>                     1441.4220 1445.5528 1448.0267<br/>                     1477.6875 1480.8073 1486.3647<br/>                     1487.3645 1492.2606 1506.0201<br/>                     1511.6949 1521.5509 1528.7786<br/>                     1711.2525 2223.5495 2946.2859<br/>                     3076.2960 3077.1846 3084.4419<br/>                     3159.5120 3164.4753 3164.7250<br/>                     3172.2161 3183.2293 3183.8993<br/>                     3187.1018 3196.2627 3221.6951</p> |
|---|--|---|

I  
 tmaG801

|   |   |  |
|---|---|--|
| b3lyp -555.8021493<br>ccscd(t) -554.3708711<br>mp2(3df,2p) -554.5416981<br>mp2(d,p) -554.2012211<br>-----<br>ZPE 0.2104286<br>Thermal 0.2217434<br>S2: 0.775445<br>-----<br>G2M(MP2,cc) Energy (OK): -554.5009195<br>G2M(MP2,cc) Enthalpy (298K): -554.4896047<br>T1 Diag: 0.02053256 | Geometry:<br>C -1.511111 1.245896 0.455316<br>C -1.629112 -0.184544 1.030563<br>C -0.266993 -0.768883 0.876249<br>H -1.933496 2.088891 0.997249<br>C -0.085883 1.382478 0.019893<br>H -2.114572 -0.349241 1.992338<br>H 0.310427 2.268904 -0.449737<br>H -0.013897 -1.782280 1.151514<br>O -2.402292 0.871630 -0.668750<br>O -3.180132 -1.301408 -0.659519<br>C -2.556463 -0.410936 -0.199463<br>C 0.556258 0.180224 0.267084<br>N 1.970616 -0.121740 -0.113576<br>C 2.669827 1.092852 -0.676287<br>C 2.740867 -0.589435 1.105144<br>C 1.980614 -1.210621 -1.171317<br>H 2.161705 1.409136 -1.584117<br>H 2.660299 1.886348 0.067558<br>H 3.695193 0.811337 -0.907134<br>H 2.282641 -1.494125 1.495148<br>H 2.712011 0.198172 1.855369<br>H 3.767433 -0.792397 0.804496<br>H 1.526626 -2.109088 -0.761547<br>H 3.014209 -1.405035 -1.454050<br>H 1.408482 -0.862402 -2.029001 | Frequencies:<br>36.5092 76.9976 141.0502<br>199.4241 220.2531 236.3097<br>277.0222 298.1424 327.6620<br>341.6871 369.4073 404.8218<br>455.5067 479.1342 496.1980<br>590.4308 597.5184 661.8760<br>687.1827 718.1190 752.3097<br>810.9428 826.6199 859.7959<br>882.5463 913.7723 931.7740<br>939.9979 952.4960 1022.3440<br>1040.4768 1074.1448 1079.2027<br>1122.9019 1135.8729 1139.4296<br>1173.6318 1231.1028 1254.7466<br>1261.7590 1269.4414 1294.3519<br>1298.3332 1318.4580 1366.8285<br>1444.2950 1445.7496 1472.8432<br>1475.1298 1483.7615 1488.6568<br>1501.4680 1504.4687 1508.2447<br>1526.1543 1929.1249 3074.2227<br>3076.7710 3082.3949 3111.9143<br>3137.4512 3167.0892 3168.4075<br>3174.6063 3179.1441 3182.0025<br>3185.0607 3230.3088 3249.6754 |
|---|---|--|

### H->I (i)

tmaG402

|   |                                 |                               |
|---|---------------------------------|-------------------------------|
| b3lyp -555.7528535                        | Geometry:                       | Frequencies:                  |
| ccsd(t) -554.3166537                      |                                 |                               |
| mp2(3df,2p) -554.470366                   | C -1.507295 1.387884 0.553658   | -657.1346 34.9987 63.6152     |
| mp2(d,p) -554.1300216                     | C -1.624932 -0.700233 0.967601  | 123.5220 201.0507 231.1272    |
| -----                                     | C -0.244330 -0.870457 0.921754  | 246.6700 267.4563 315.4635    |
| ZPE 0.2079844                             | H -1.908003 2.139858 1.226023   | 334.2125 345.0986 366.9650    |
| Thermal 0.2193877                         | C -0.087405 1.373594 0.154212   | 406.4462 453.3499 467.3024    |
| S2: 0.7908                                | H -2.171494 -1.257934 1.724584  | 497.0063 531.9837 589.0953    |
| -----                                     | H 0.364496 2.272841 -0.245281   | 600.4105 647.2487 721.5733    |
| G2M(MP2,cc) Energy (OK): -554.4490137     | H 0.232670 -1.604197 1.561359   | 743.9070 778.9497 823.0047    |
| G2M(MP2,cc) Enthalpy (298K): -554.4376104 | O -2.389451 0.980446 -0.456918  | 843.1416 866.5598 910.6389    |
| T1 Diag: 0.03053089                       | O -3.127035 -1.121004 -0.895746 | 938.1275 952.7826 972.3109    |
|   | C -2.475123 -0.372051 -0.249042 | 1008.9637 1073.8923 1097.1753 |
|   | C 0.518583 0.169441 0.277380    | 1106.6757 1131.7433 1133.8848 |
|   | N 1.933202 -0.095415 -0.142330  | 1142.0818 1195.5399 1246.2316 |
|   | C 2.578150 1.111656 -0.778367   | 1254.5858 1292.7293 1312.3695 |
|   | C 2.767638 -0.493916 1.059841   | 1351.5261 1397.6081 1441.3485 |
|   | C 1.936349 -1.224888 -1.156862  | 1443.7166 1448.4667 1474.8193 |
|   | H 2.003061 1.405297 -1.653452   | 1483.5731 1487.2034 1490.1870 |
|   | H 2.619922 1.921080 -0.053170   | 1503.5100 1510.2595 1525.1139 |
|   | H 3.586759 0.832184 -1.075899   | 1592.6367 1894.3256 3071.7681 |
|   | H 2.380478 -1.417265 1.480938   | 3077.1572 3082.6746 3148.8355 |
|   | H 2.719801 0.307193 1.794637    | 3165.7109 3167.4098 3172.1929 |
|   | H 3.793170 -0.645980 0.727695   | 3173.6835 3176.0565 3176.8780 |
|   | H 1.501001 -2.111132 -0.701733  | 3179.7671 3190.2484 3198.0283 |
|   | H 2.966262 -1.417466 -1.453976  |                               |
|   | H 1.341536 -0.918290 -2.015152  |                               |

**H->N (ii)**

tmaG502

|   |                                 |                               |
|---|---------------------------------|-------------------------------|
| b3lyp -555.771207                         | Geometry:                       | Frequencies:                  |
| ccsd(t) -554.3326411                      |                                 |                               |
| mp2(3df,2p) -554.4977405                  | C 0.212674 -1.266121 -0.548973  | -175.4684 21.1493 35.8031     |
| mp2(d,p) -554.1620758                     | C 1.512283 -1.704671 -0.401504  | 77.6976 118.6898 143.9046     |
| -----                                     | C 2.574408 -1.200108 0.529449   | 194.3045 208.6946 252.9831    |
| ZPE 0.2052474                             | C -0.390212 -0.152331 0.051001  | 278.8320 314.3392 340.9914    |
| Thermal 0.2182126                         | C 0.290657 1.001875 0.597783    | 350.0436 371.0659 396.7098    |
| S2: 0.775874                              | C 1.270108 1.628561 -0.061975   | 425.2782 452.8847 460.0289    |
| -----                                     | H -0.393606 -1.885111 -1.197929 | 522.9941 553.2297 581.5680    |
| G2M(MP2,cc) Energy (OK): -554.4630584     | H 1.811270 -2.580692 -0.972070  | 604.1296 662.5423 711.3854    |
| G2M(MP2,cc) Enthalpy (298K): -554.4500932 | H 2.606356 -1.694496 1.522686   | 800.2014 846.2406 891.3923    |
| T1 Diag: 0.02172325                       | H 0.034428 1.461430 1.546914    | 929.5917 936.5377 951.2560    |
|   | O 2.102633 2.189934 -0.610959   | 985.6176 1040.7528 1067.8945  |
|   | O 3.389150 -0.368651 0.221722   | 1119.8410 1126.8682 1150.4855 |
|   | N -1.915651 -0.037374 0.029975  | 1217.3188 1246.3150 1252.9706 |
|   | C -2.416451 0.237524 1.433648   | 1275.3159 1341.9786 1395.9241 |
|   | C -2.334032 1.103176 -0.877128  | 1421.8575 1438.3952 1439.4230 |
|   | C -2.607742 -1.291945 -0.445794 | 1463.1990 1473.6212 1478.9344 |
|   | H -2.082267 -0.567280 2.085712  | 1484.9065 1489.6011 1493.5362 |
|   | H -2.032748 1.192988 1.778410   | 1505.8443 1513.8529 1531.1501 |
|   | H -3.504027 0.277112 1.407930   | 1783.5498 2244.7477 2898.9912 |
|   | H -1.984144 0.888067 -1.885054  | 3072.1832 3076.8168 3083.1315 |
|   | H -1.883189 2.022947 -0.514935  | 3149.0773 3155.3430 3162.4664 |
|   | H -3.420528 1.179861 -0.860876  | 3164.1090 3170.8769 3180.1538 |
|   | H -2.385592 -1.460258 -1.496136 | 3181.9535 3187.3836 3192.3539 |
|   | H -3.679133 -1.143036 -0.327363 |                               |
|   | H -2.281683 -2.135940 0.157727  |                               |

**N->->M (iii)**

tmaE801

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| <p>b3lyp -555.7720544<br/>                     ccscd(t) -554.3276471<br/>                     mp2(3df,2p) -554.4826153<br/>                     mp2(d,p) -554.1440301<br/>                     -----<br/>                     ZPE 0.2062659<br/>                     Thermal 0.2186718<br/>                     S2: 0.757495<br/>                     -----<br/>                     G2M(MP2,cc) Energy (0K): -554.4599664<br/>                     G2M(MP2,cc) Enthalpy (298K): -554.4475605<br/>                     T1 Diag: 0.03615586</p> | <p>Geometry:</p> <p>C -1.380740 -1.750305 -0.593967<br/>                     C -2.140481 -1.041942 0.326458<br/>                     C -1.539227 1.351448 -0.625447<br/>                     C -0.036213 -1.392414 -0.781617<br/>                     C 0.381874 -0.223170 -0.171852<br/>                     C -0.609722 0.666985 0.315921<br/>                     H -1.856285 -2.594851 -1.080241<br/>                     H -0.465587 1.230181 1.233883<br/>                     H 0.601423 -2.054558 -1.350496<br/>                     O -3.085774 -0.833110 0.957092<br/>                     O -2.177301 2.323257 -0.307627<br/>                     H -1.585523 0.928580 -1.648325<br/>                     N 1.840409 0.052788 0.108377<br/>                     C 2.757525 -0.910456 -0.603329<br/>                     C 2.189848 1.457184 -0.346198<br/>                     C 2.094511 -0.067790 1.599714<br/>                     H 2.573809 -1.920192 -0.243876<br/>                     H 2.585716 -0.843261 -1.675634<br/>                     H 3.782850 -0.624630 -0.377498<br/>                     H 1.562547 2.169393 0.183051<br/>                     H 2.010339 1.527916 -1.417289<br/>                     H 3.239840 1.639735 -0.122963<br/>                     H 1.482039 0.658273 2.127420<br/>                     H 3.148603 0.133027 1.786149<br/>                     H 1.837715 -1.077535 1.913356</p> | <p>Frequencies:</p> <p>-386.6235 44.4665 79.5706<br/>                     89.5180 147.7839 193.5397<br/>                     226.2878 244.7963 274.3375<br/>                     287.3146 308.3036 330.6278<br/>                     335.8296 356.0895 379.6923<br/>                     425.8676 445.2519 513.2277<br/>                     534.0949 567.6834 606.3780<br/>                     676.9887 727.1176 802.2717<br/>                     843.1946 899.0040 918.0777<br/>                     935.0102 949.4465 957.1840<br/>                     1010.8390 1040.2940 1071.8975<br/>                     1120.6629 1125.1024 1131.0565<br/>                     1140.0970 1248.9240 1253.2216<br/>                     1281.3384 1309.2877 1368.9881<br/>                     1412.4762 1442.1540 1442.7350<br/>                     1460.4834 1474.7727 1484.9156<br/>                     1486.4446 1491.6304 1503.7639<br/>                     1509.7820 1524.9164 1527.0719<br/>                     1753.1957 2077.5697 2918.1569<br/>                     3073.0793 3074.1024 3080.1855<br/>                     3152.8017 3164.5711 3164.8396<br/>                     3171.4407 3175.7266 3180.6423<br/>                     3184.5810 3185.9621 3221.5934</p> |
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**N->->X (iv)**

tmaE707

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|---|---|--|
| b3lyp -555.7508695<br>ccsd(t) -554.3091702<br>mp2(3df,2p) -554.4731926<br>mp2(d,p) -554.1329553<br>-----<br>ZPE 0.2065995<br>Thermal 0.2189775<br>S2: 0.76194<br>-----<br>G2M(MP2,cc) Energy (OK): -554.4428080<br>G2M(MP2,cc) Enthalpy (298K): -554.4304300<br>T1 Diag: 0.02456716 | Geometry:<br>C 1.681915 1.373515 -0.162223<br>C 2.449364 -0.594730 -0.332827<br>C 0.204941 -1.185437 0.472905<br>C 1.511517 -1.480579 0.339338<br>C -0.441246 0.032641 -0.007745<br>C 0.212164 1.125832 -0.420909<br>H 1.902179 -2.443819 0.656029<br>H 2.254179 1.777323 -1.010909<br>H -0.406726 -1.941813 0.949084<br>H -0.295845 1.958033 -0.893945<br>O 2.051800 1.538776 1.009330<br>O 3.586486 -0.666035 -0.603252<br>N -1.959630 -0.035641 -0.059930<br>C -2.582676 1.207668 -0.647870<br>C -2.406409 -1.209889 -0.908883<br>C -2.497283 -0.181836 1.352822<br>H -2.317373 2.069597 -0.040487<br>H -2.243289 1.334696 -1.673161<br>H -3.661855 1.070315 -0.635524<br>H -2.035831 -2.137061 -0.481472<br>H -2.008823 -1.078517 -1.913423<br>H -3.494804 -1.224842 -0.929689<br>H -2.140292 -1.109590 1.790531<br>H -3.584993 -0.195098 1.305659<br>H -2.149122 0.665228 1.940546 | Frequencies:<br>-369.4832 53.6549 62.8087<br>84.3552 141.9364 198.4228<br>208.5349 247.4958 262.9856<br>264.6619 325.9669 354.5504<br>365.0324 383.9482 401.2553<br>406.9613 460.7861 474.5631<br>503.2217 601.2822 639.3494<br>669.2847 769.8372 812.8529<br>826.7042 884.4468 914.7643<br>939.7183 950.8635 981.1144<br>989.5842 1030.4484 1057.2854<br>1071.5193 1133.9171 1139.8819<br>1222.1557 1251.1548 1253.6041<br>1283.6264 1329.3399 1363.7696<br>1422.2553 1444.0520 1445.9961<br>1477.5060 1486.1217 1486.7494<br>1491.4496 1506.6419 1509.8671<br>1511.6050 1527.7421 1620.8220<br>1682.5411 1947.3712 2987.4107<br>3076.2110 3076.4337 3083.1909<br>3153.3526 3165.6404 3166.8495<br>3173.1672 3179.6320 3181.0705<br>3183.6114 3185.8738 3195.8917 |
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